Dynamics: A Set of Notes on Theoretical Physical Chemistry

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Chapter 1

Vector Calculus

These are summary notes on vector analysis and vector calculus. The purpose is to serve as a *review*. Although the discussion here can be generalized to differential forms and the introduction to tensors, transformations and linear algebra, an in depth discussion is deferred to later chapters, and to further reading.[1,2,3,4,5]

For the purposes of this review, it is assumed that *vectors* are *real* and represented in a *3-dimensional Cartesian basis* $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$, unless otherwise stated. Sometimes the generalized coordinate notation x_1, x_2, x_3 will be used generically to refer to x, y, z Cartesian components, respectively, in order to allow more concise formulas to be written using using i, j, k indexes and cyclic permutations.

If a sum appears without specification of the index bounds, assume summation is over the entire range of the index.

1.1 Properties of vectors and vector space

A **vector** is an entity that exists in a **vector space**. In order to take for (in terms of numerical values for it's components) a vector must be associated with a **basis** that spans the vector space. In 3-D space, for example, a Cartesian basis can be defined $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$. This is an example of an **orthonormal basis** in that each component basis vector is normalized $\hat{\mathbf{x}} \cdot \hat{\mathbf{x}} = \hat{\mathbf{y}} \cdot \hat{\mathbf{y}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{z}} = 1$ and orthogonal to the other basis vectors $\hat{\mathbf{x}} \cdot \hat{\mathbf{y}} = \hat{\mathbf{y}} \cdot \hat{\mathbf{z}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{x}} = 0$. More generally, a basis (not necessarily the Cartesian basis, and not necessarily an orthonormal basis) is denoted $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. If the basis is normalized, this fact can be indicated by the "hat" symbol, and thus designated $(\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$.

Here the properties of *vectors* and the *vector space* in which they reside are summarized. Although the present chapter focuses on vectors in a 3-dimensional (3-D) space, many of the properties outlined here are more general, as will be seen later. Nonetheless, in chemistry and physics, the specific case of vectors in 3-D is so prevalent that it warrants special attention, and also serves as an introduction to more general formulations.

A **3-D vector** is defined as an entity that has both magnitude and direction, and can be characterized, provided a basis is specified, by an ordered triple of numbers. The vector $\mathbf{x}$, then, is represented as $\mathbf{x} = (x_1, x_2, x_3)$.

Consider the following definitions for operations on the vectors $\mathbf{x}$ and $\mathbf{y}$ given by $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3)$:

1. Vector equality: $\mathbf{x} = \mathbf{y}$ if $x_i = y_i \ \forall\, i = 1, 2, 3$

2. Vector addition: $\mathbf{x} + \mathbf{y} = \mathbf{z}$ if $z_i = x_i + y_i \ \forall\, i = 1, 2, 3$

3. Scalar multiplication: $a\mathbf{x} = (ax_1, ax_2, ax_3)$

4. Null vector: There exists a unique null vector $\mathbf{0} = (0, 0, 0)$

Furthermore, assume that the following properties hold for the above defined operations:

1. Vector addition is commutative and associative:
$\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$
$(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$

2. Scalar multiplication is associative and distributive:
$(ab)\mathbf{x} = a(b\mathbf{x})$
$(a + b)(\mathbf{x} + \mathbf{y}) = a\mathbf{x} + b\mathbf{x} + a\mathbf{y} + b\mathbf{y}$

The collection of all 3-D vectors that satisfy the above properties are said to form a **3-D vector space**.

1.2 Fundamental operations involving vectors

The following fundamental vector operations are defined.

Scalar Product:

$$\begin{aligned} \mathbf{a} \cdot \mathbf{b} &= a_x b_x + a_y b_y + a_z b_z = \sum_i a_i b_i = |\mathbf{a}||\mathbf{b}| cos(\theta) \\ &= \mathbf{b} \cdot \mathbf{a} \end{aligned} \tag{1.1}$$

where $|\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}}$, and θ is the angle between the vectors $\mathbf{a}$ and $\mathbf{b}$.

Cross Product:

$$\mathbf{a} \times \mathbf{b} = \hat{\mathbf{x}}(a_y b_z - a_z b_y) + \hat{\mathbf{y}}(a_z b_x - a_x b_z) + \hat{\mathbf{z}}(a_x b_y - a_y b_x) \tag{1.2}$$

or more compactly

$$\mathbf{c} = \mathbf{a} \times \mathbf{b} \tag{1.3}$$

$$where \tag{1.4}$$

$$c_i = a_j b_k - a_k b_j \tag{1.5}$$

where i, j, k are x, y, z and the cyclic permutations z, x, y and y, z, x, respectively. The cross product can be expressed as a determinant:

The norm of the cross product is

$$|\mathbf{a} \times \mathbf{b}| = |\mathbf{a}||\mathbf{b}| sin(\theta) \tag{1.6}$$

where, again, θ is the angle between the vectors $\mathbf{a}$ and $\mathbf{b}$ The cross product of two vectors $\mathbf{a}$ and $\mathbf{b}$ results in a vector that is perpendicular to both $\mathbf{a}$ and $\mathbf{b}$, with magnitude equal to the area of the parallelogram defined by $\mathbf{a}$ and $\mathbf{b}$.

The *Triple Scalar Product*:

$$\mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = \mathbf{c} \cdot \mathbf{a} \times \mathbf{b} = \mathbf{b} \cdot \mathbf{c} \times \mathbf{a} \tag{1.7}$$

and can also be expressed as a determinant

The triple scalar product is the volume of a parallelopiped defined by $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$.

The *Triple Vector Product*:

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b}) \tag{1.8}$$

The above equation is sometimes referred to as the $BAC - CAB$ rule.

Note: the parenthases need to be retained, i.e. $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) \neq (\mathbf{a} \times \mathbf{b}) \times \mathbf{c}$ in general.

Lattices/Projection of a vector

$$\mathbf{a} = (a_x)\hat{\mathbf{x}} + (a_y)\hat{\mathbf{y}} + (a_y)\hat{\mathbf{y}} \tag{1.9}$$

$$\mathbf{a} \cdot \hat{\mathbf{x}} = a_x \tag{1.10}$$

$$\mathbf{r} = r_1 \mathbf{a_1} + r_2 \mathbf{a_2} + r_3 \mathbf{a_3} \tag{1.11}$$

$$\mathbf{a_i} \cdot \mathbf{a_j} = \delta_{ij} \tag{1.12}$$

$$\mathbf{a_i} = \frac{\mathbf{a_j} \times \mathbf{a_k}}{\mathbf{a_i} \cdot (\mathbf{a_j} \times \mathbf{a_k})} \tag{1.13}$$

Gradient, ∇

$$\nabla = \hat{\mathbf{x}} \left[\frac{\partial}{\partial x} \right] + \hat{\mathbf{y}} \left[\frac{\partial}{\partial y} \right] + \hat{\mathbf{z}} \left[\frac{\partial}{\partial z} \right] \tag{1.14}$$

$$\nabla f(|\mathbf{r}|) = \hat{\mathbf{r}} \left[\frac{\partial f}{\partial r} \right] \tag{1.15}$$

$$d\mathbf{r} = \hat{\mathbf{x}} dx + \hat{\mathbf{y}} dy + \hat{\mathbf{z}} dz \tag{1.16}$$

$$d\varphi = (\nabla \varphi) \cdot d\mathbf{r} \tag{1.17}$$

$$\nabla(uv) = (\nabla u)v + u(\nabla v) \tag{1.18}$$

Divergence, $\nabla \cdot$

$$\nabla \cdot \mathbf{V} = \left[\frac{\partial V_x}{\partial x} \right] + \left[\frac{\partial V_y}{\partial y} \right] + \left[\frac{\partial V_z}{\partial z} \right] \tag{1.19}$$

$$\nabla \cdot \mathbf{r} = 3 \tag{1.20}$$

$$\nabla \cdot (\mathbf{r} f(r)) = 3f(r) + r \frac{df}{dr} \tag{1.21}$$

if $f(r) = r^{n-1}$ then $\nabla \cdot \hat{\mathbf{r}} r^n = (n+2) r^{n-1}$

$$\nabla \cdot (f\mathbf{v}) = \nabla f \cdot \mathbf{v} + f \nabla \cdot \mathbf{v} \tag{1.22}$$

Curl,$\nabla \times$

$$\hat{\mathbf{x}}(\left[\frac{\partial V_z}{\partial y} \right] - \left[\frac{\partial V_y}{\partial z} \right]) + \hat{\mathbf{y}}(\left[\frac{\partial V_x}{\partial z} \right] - \left[\frac{\partial V_z}{\partial x} \right]) + \hat{\mathbf{z}}(\left[\frac{\partial V_y}{\partial x} \right] - \left[\frac{\partial V_x}{\partial y} \right]) \tag{1.23}$$

$$\nabla \times (f\mathbf{v}) = f \nabla \times \mathbf{v} + (\nabla f) \times \mathbf{v} \tag{1.24}$$

$$\nabla \times \mathbf{r} = 0 \tag{1.25}$$

$$\nabla \times (\mathbf{r} f(r)) = 0 \tag{1.26}$$

$$\nabla(\mathbf{a} \cdot \mathbf{b}) = (\mathbf{b} \cdot \boldsymbol{\nabla})\mathbf{a} + (\mathbf{a} \cdot \boldsymbol{\nabla})\mathbf{b} + \mathbf{b} \times (\nabla \times \mathbf{a}) + \mathbf{a} \times (\nabla \times \mathbf{b}) \tag{1.27}$$

$$\nabla \cdot \nabla = \nabla \times \nabla = \nabla^2 = \left[\frac{\partial^2}{\partial^2 x}\right] + \left[\frac{\partial^2}{\partial^2 y}\right] + \left[\frac{\partial^2}{\partial^2 z}\right] \tag{1.28}$$

Vector Integration

Divergence theorem (Gauss's Theorem)

$$\int_V \nabla \cdot \mathbf{f}(\mathbf{r}) d^3r = \int_S \nabla \cdot \mathbf{f}(\mathbf{r}) \cdot d\boldsymbol{\sigma} = \int_S \nabla \cdot \mathbf{f}(\mathbf{r}) \cdot \underline{n} da \tag{1.29}$$

let $\mathbf{f}(\mathbf{r}) = u\nabla v$ then

$$\nabla \cdot (u\nabla v) = \nabla u \cdot \nabla v + u\nabla^2 v \tag{1.30}$$

$$\int_V \nabla u \cdot \nabla v d^3r + \int_V u\nabla^2 v d^3r = \int_S (u\nabla v) \cdot \underline{n} da \tag{1.31}$$

The above gives the second form of Green's theorem.

Let $\mathbf{f}(\mathbf{r}) = u\nabla v - v\nabla u$ then

$$\int_V \nabla u \cdot \nabla v d^3r + \int_V u\nabla^2 v d^3r - \int_V \nabla u \cdot \nabla v d^3r - \int_V v\nabla^2 u d^3r = \int_S (u\nabla v) \cdot \underline{n} da - \int_S (v\nabla u) \cdot \underline{n} da \tag{1.32}$$

Above gives the first form of Green's theorem.

Generalized Green's theorem

$$\int_V u\hat{L}u - u\hat{L}v d^3r = \int_S p(v\nabla u - u\nabla v)) \cdot \underline{n} da \tag{1.33}$$

where $\hat{L}$ is a self-adjoint (Hermetian) "Sturm-Lioville" operator of the form:

$$\hat{L} = \nabla \cdot [p\nabla] + q \tag{1.34}$$

Stokes Theorem

$$\int_S (\nabla \times \mathbf{v}) \cdot \underline{n} da = \oint_C \mathbf{V} \cdot d\boldsymbol{\lambda} \tag{1.35}$$

Generalized Stokes Theorem

$$\int_S (d\boldsymbol{\sigma} \times \nabla) \circ [] = \oint_C d\boldsymbol{\lambda} \circ [] \tag{1.36}$$

where $\circ = \_, \cdot, \times$

Vector Formulas

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}) \tag{1.37}$$

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c} \tag{1.38}$$

$$(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}) \tag{1.39}$$

$$\nabla \times \nabla \psi = 0 \tag{1.40}$$

$$\nabla \cdot (\nabla \times \mathbf{a}) = 0 \tag{1.41}$$

$$\nabla \times (\nabla \times \mathbf{a}) = \nabla(\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a} \tag{1.42}$$

$$\nabla \cdot (\psi \mathbf{a}) = \mathbf{a} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{a} \tag{1.43}$$

$$\nabla \times (\psi \mathbf{a}) = \nabla \psi \times \mathbf{a} + \psi \nabla \times \mathbf{a} \tag{1.44}$$

$$\nabla(\mathbf{a} \cdot \mathbf{b}) = (\mathbf{a} \cdot \nabla)\mathbf{b} + (\mathbf{b} \cdot \nabla)\mathbf{a} + \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a}) \tag{1.45}$$

$$\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b}) \tag{1.46}$$

$$\nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{a}(\nabla \cdot \mathbf{b}) - \mathbf{b}(\nabla \cdot \mathbf{a}) + (\mathbf{b} \cdot \nabla)\mathbf{a} - (\mathbf{a} \cdot \nabla)\mathbf{b} \tag{1.47}$$

If $\mathbf{x}$ is the coordinate of a point with magnitude $r = |\mathbf{x}|$, and $\mathbf{n} = \mathbf{x}/r$ is a unit radial vector

$$\nabla \cdot \mathbf{x} = 3 \tag{1.48}$$

$$\nabla \times \mathbf{x} = 0 \tag{1.49}$$

$$\nabla \cdot \mathbf{n} = 2/r \tag{1.50}$$

$$\nabla \times \mathbf{n} = 0 \tag{1.51}$$

$$(\mathbf{a} \cdot \nabla)\mathbf{n} = (1/r)[\mathbf{a} - \mathbf{n}(\mathbf{a} \cdot \mathbf{n})] \tag{1.52}$$

Chapter 2

Linear Algebra

2.1 Matrices, Vectors and Scalars

Matrices - 2 indexes (2^{nd} rank tensors) - $A_{ij}/\mathbf{A}$
Vectors - 1 index* (1^{st} rank tensor) - $a_i/\mathbf{a}$
Scalar - 0 index* (0 rank tensor) - a

Note: for the purpose of writing linear algebraic equations, a vector can be written as an $N \times 1$ "Column vector " (a type of matrix), and a scalar as a 1×1 matrix.

2.2 Matrix Operations

Multiplication by a scalar α.

$$\underbrace{\mathbf{C}}_{N\times N} = \underbrace{\alpha\mathbf{A}}_{N\times N} = \mathbf{A}\alpha \qquad \text{means} \qquad C_{ij} = \alpha A_{ij} = A_{ij}\cdot\alpha$$

Addition/Subtraction

$$\mathbf{C} = \mathbf{A} - \mathbf{B} = \mathbf{B} - \mathbf{A} \qquad \text{means} \qquad C_{ij} = A_{ij} - B_{ij}$$

Multiplication (inner product)

$$\underbrace{\mathbf{C}}_{N\times N} = \underbrace{\mathbf{A}\,\mathbf{B}}_{N\times M\cdot M\times N} \qquad \text{means} \qquad C_{ij} = \sum_k A_{ik}B_{kj}$$

$$\mathbf{AB} \neq \mathbf{BA} \qquad \text{in general}$$

$$\mathbf{A}\cdot(\mathbf{B}\cdot\mathbf{C}) = (\mathbf{AB})\mathbf{C} = \mathbf{ABC} \qquad \text{associative, not always communitive}$$

Multiplication (outer product/direct product)

$$\underbrace{\mathbf{C}}_{nm\times nm} = \mathbf{A}\otimes\mathbf{B} \qquad \text{means} \qquad C_{\alpha\beta} = A_{ij}B_{k\ell}$$

$$\alpha = n(i-1)+k \qquad\qquad \beta = m(j-1)+\ell$$

$$\mathbf{A} \otimes \mathbf{B} \neq \mathbf{B} \otimes \mathbf{A} \qquad \mathbf{A} \otimes (\mathbf{B} \otimes \mathbf{C}) = (\mathbf{A} \otimes \mathbf{B})\mathbf{C}$$

Note, for "vectors"

$$\mathbf{C} = \underbrace{\mathbf{a} \otimes \mathbf{b}^T}_{N\times 1 \cdot 1\times N} \qquad \text{means} \qquad C_{ij} = a_i b_j$$

2.3 Transpose of a Matrix

$$\underbrace{\mathbf{A} = \mathbf{B}^T}_{N\times M \quad (M\times N)^T = N\times M} \qquad \text{means} \qquad A_{ij} = (B_{ij})^T = B_{ji}$$

Note:

$$(\mathbf{A}^T)^T = \mathbf{A} \left[(A_{ij})^T\right]^T = [A_{ji}]^T = A_{ij}$$

$$(\mathbf{A} \cdot \mathbf{B})^T = \mathbf{B}^T \cdot \mathbf{A}^T$$

$$\begin{aligned} \mathbf{C} &= (\mathbf{A} \cdot \mathbf{B})^T = \mathbf{B}^T \cdot \mathbf{A}^T \\ C_{ij} &= \left(\sum_k A_{ik} B_{kj}\right)^T = \sum_k A_{jk} B_{ki} \\ &= \sum_k B_{ki} A_{jk} = \sum_k (B_{ik})^T (A_{kj})^T \end{aligned}$$

2.4 Unit Matrix

(identity matrix)

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathbf{1} \tag{2.1}$$

$$1_{ij} \equiv \delta_{ij}$$

$$\mathbf{1}^{-1} = \mathbf{1}^T = \mathbf{1} \qquad \mathbf{A}\mathbf{1} = \mathbf{1}\mathbf{A} = \mathbf{A}$$

Commutator: a linear operation

$$[\mathbf{A}, \mathbf{B}] \equiv \mathbf{A}\mathbf{B} - \mathbf{B}\mathbf{A}$$

$$[\mathbf{A}, \mathbf{B}] = 0 \qquad \text{if } \mathbf{A} \text{ and } \mathbf{B} \text{ are diagonal matrices}$$

Diagonal Matrices:

$$A_{ij} = a_{ii}\delta_{ij}$$

Jacobi Identity:

$$[A, [B, C]] = [B, [A, C]] - [C, [A, B]]$$

2.5 Trace of a (Square) Matrix

(a linear operator)

$$T_r(\mathbf{A}) = \sum_i A_{ii} = T_r\left(\mathbf{A}^T\right)$$

$$\begin{aligned} T_r(\mathbf{A}\cdot\mathbf{B}) = T_r(\mathbf{C}) &= \sum_i C_{ii} = \sum_i \sum_k A_{ik}B_{ki} \\ &= \sum_k \sum_i B_{ki}A_{ik} = T_r(\mathbf{BA}) \end{aligned}$$

Note $T_r([\mathbf{A},\mathbf{B}]) = 0$

$$T_r(\alpha\mathbf{A} + \beta\mathbf{B}) = \alpha T_r(\mathbf{A}) + \beta T_r(\mathbf{B})$$

2.5.1 Inverse of a (Square) Matrix

$$\mathbf{A}^{-1}\cdot\mathbf{A} = \mathbf{1} = \mathbf{A}\cdot\mathbf{A}^{-1}$$

Note $\mathbf{1}\cdot\mathbf{1} = \mathbf{1}$, thus $\mathbf{1} = \mathbf{1}^{-1}$

$(\mathbf{A}\cdot\mathbf{B})^{-1} = \mathbf{B}^{-1}\cdot\mathbf{A}^{-1}$ prove

2.6 More on Trace

$$\begin{aligned}
&Tr(ABC) = Tr(CBA) \\
&Tr(a\otimes b^T) = a^T\cdot b \\
&Tr(U^+AU) = Tr(A) \quad U^+U = 1 \text{ or } \quad Tr(B^{-1}AB) = Tr(A) \\
&Tr(S^+S) \geq 0 \qquad Tr(BSB^{-1}BTB^{-1} = Tr(ST) \\
&Tr(A) = TrA^+ \qquad Tr(S'T') \\
&Tr(AB) = Tr(BA) = Tr(B^+A^+) \\
&Tr(ABC) = Tr(CAB) = Tr(BCA) \\
&Tr([A,B]) = 0 \\
&Tr(AB) = 0 \text{ if } A = A^T \text{ and } B = B^T
\end{aligned}$$

2.7 More on $[A, B]$

$$[S_x, S_y] = iS_z$$

Proof: $(\mathbf{A}\cdot\mathbf{B})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
If $\mathbf{x}\cdot\mathbf{y} = 1$ then $\mathbf{y} = \mathbf{x}^{-1}$
associative $(\mathbf{A}\cdot\mathbf{B})\cdot(\mathbf{B}^{-1}\cdot\mathbf{A}^{-1}) = \mathbf{A}\cdot(\mathbf{B}\cdot\mathbf{B}^{-1})\cdot\mathbf{A}^{-1} = (\mathbf{A}\cdot\mathbf{A}^{-1}) = 1$ thus $(\mathbf{B}^{-1}\cdot\mathbf{A}^{-1}) = (\mathbf{A}\cdot\mathbf{B})^{-1}$

2.8 Determinants

$$det(\mathbf{A}) = \begin{vmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \ddots & \vdots & A_{nn} \end{vmatrix} = \sum_{i,k\ldots} \epsilon_{ijk\ldots} A_{1i} A_{2j} A_{3k} \ldots \tag{2.2}$$

$\epsilon_{ijk\ldots}$: Levi-Civita symbol (± 1 even/odd permutation of $1, 2, 3 \ldots$, otherwise 0. (has $N!$ terms)
A is a square matrix, ($N \times N$)

2.8.1 Laplacian expansion

$$\begin{aligned} D &= \sum_i^N (-1)^{i+j} M_{ij} A_{ij} \\ &= \sum_i^N c_{ij} A_{ij} \end{aligned}$$

$$\begin{aligned} M_{ij} &= \text{“minor” } ij \\ c_{ij} &= \text{“cofactor” } = (-1)^{i+j} M_{ij} \end{aligned}$$

$$D = \pi_k A_{kk} \tag{2.3}$$

$$\begin{vmatrix} A_{11} & 0 \\ A_{21} & A_{22} \\ - & - \end{vmatrix} \tag{2.4}$$

$$\sum_i^N = A_{ij} c_{ik} = det(A) \delta_{jk} = \sum A_{ji} c_{ik}$$

$det(A)$ is an antisymmetrized product

Properties: for an $N \times N$ matrix A

1. The value of $det(A) = 0$ if
   - any two rows (or columns) are equal
   - each element of a row (or column) is zero
   - any row (or column) can be represented by a linear combination of the other rows (or columns). In this case, A is called a “singular” matrix, and will have one or more of it’s eigenvalues equal to zero.
2. The value of $det(A)$ is unchanged if
   - two rows (or columns) are swapped, sign changes
   - a multiple of one row (or column) is added to another row (or column)
   - A is transposed $det(A) = det(A^+)$ or $det(A^+) = det(A^*) = (det(A))^*$

- A undergoes unitary transformation $det(A) = det(U^{+}AU)$ (including the unitary tranformation that diagonalized A)

$$det(e^{A}) = e^{tr(A)} \tag{2.5}$$

3. If any row (or column) of A is multiplied by a scalar α, the value of the determinat is $\alpha det(A)$. If the whole matrix is multiplied by α, then

$$det(\alpha A) = \alpha^{N} det(A) \tag{2.6}$$

4. If $A = BC$, $det(A) = det(B) \times det(C)$, but if $A = B + C$, $det(A) \neq det(B) + det(C)$. ($det(A)$ is not a linear operator)

$$det(A^{N}) = [det(A)]^{N} \tag{2.7}$$

5. If A is diagonalized, $det(A) = \Pi_i A_{ii}$ (also, $det(\mathbf{1}) = 1$)
6. $det(A)^{-1}) = (det(A))^{-1}$
7. $det(A^{*}) = (detA)^{*} = det(A^{+})$
8. $det(A) = det(U^{+}AU) \quad U^{+}U = 1$

2.8.2 Applications of Determinants

Wave function:

$$\Psi_{\frac{HF}{DFT}}(\mathbf{x}_1, \mathbf{x}_2 \cdots \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\mathbf{x}_1) & \psi_2(\mathbf{x}_1) & \cdots & \psi_N(\mathbf{x}_1 \\ \psi_1(\mathbf{x}_2) & \psi_2(\mathbf{x}_2) & \cdots & \vdots \\ \vdots & & \ddots & \psi_N(\mathbf{x}_N) \end{vmatrix} \tag{2.8}$$

Evaluate:

$$\int \Psi^{*}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) d\tau$$

(write all the terms). How does this expression reduce if $\int \psi_i(\mathbf{x})\psi_j(\mathbf{x}) d\tau = \delta_{iJ}$ (orthonormal spin orbitals)

J=Jacobian $|dx_k >= J|dq_j >= \sum_i |dq_i >< dq_i|dx_k >$

$$dx_1 dx_2 dx_3 = det(J) dq_1 dq_2 dq_3, \quad J_{ik} = \frac{\partial x_i}{\partial q_k}$$

$$J\left(\frac{x}{q}\right) : J_{ij} = \frac{\partial x_i}{\partial q_j}$$

$$J\left(\frac{q}{x}\right)_{ij} = \frac{\partial q_i}{\partial x_j} \tag{2.9}$$

$$det\left[J\left(\frac{q}{x}\right)\right] = \begin{vmatrix} \frac{\partial q_1}{\partial x_1} & \frac{\partial q_1}{\partial x_2} & \cdots \\ \vdots & & \ddots \end{vmatrix} \tag{2.10}$$

$$q_1 = 2x \qquad q_2 = y \qquad q_3 = z$$

$$dxdydz = \frac{1}{2} dq_1 \tag{2.11}$$

$$x' + 2x \qquad \frac{\partial x}{\partial x'} = \frac{1}{2} \qquad \frac{\partial x'}{\partial x} = 2 \qquad dx = \frac{1}{2} dx'$$

$$dx = \frac{dx}{dq_1} dq_1 = \frac{1}{2} dq_1 \tag{2.12}$$

2.9 Generalized Green's Theorem

Use:

$$\int_v \nabla \cdot v d\tau = \int_s \mathbf{v} \cdot d\boldsymbol{\sigma} \tag{2.13}$$

$$\int_v (vLu - uLv) d\tau = \int_s p(x\nabla u - u\nabla v) \cdot d\sigma \tag{2.14}$$

$$L = \nabla \cdot [p\nabla] + q = \nabla p \cdot \nabla + p\nabla^2 + q$$

$$\int_v \left[v(\nabla p \cdot \nabla u + \nabla^2 u + q)u - u(\nabla p \cdot \nabla v + p\nabla^2 v + q)v \right] d\tau$$

Note $\int vqu \, d\tau = \int uqv \, d\tau$

$$\begin{aligned} &\int_v (v\nabla \cdot [p\nabla]u + \nabla v \cdot (p\nabla u) - u\nabla \cdot [p\nabla]v - \nabla v \cdot (p\nabla u)) \, d\tau \\ &= \int_v (\nabla \cdot vp\nabla u - \nabla \cdot up\nabla v) \, d\tau \end{aligned} \tag{2.15}$$

$$\begin{aligned} &\nabla v \cdot p\nabla u + v\nabla \cdot [p\nabla]u - \nabla u \cdot p\nabla v - u\nabla \cdot [p\nabla]v \\ &= \int_s (vp\nabla u - up\nabla v) \cdot d\boldsymbol{\sigma} \\ &= \int_s p(v\nabla u - u\nabla v) \cdot d\mathbf{s} \end{aligned}$$

$$\begin{aligned} dF_i = \sum_k \frac{\partial F_i}{\partial x_k} dx_k + \frac{\partial F_i}{t} dt =& (d\mathbf{r} \cdot \nabla) F_i + \frac{\partial F_i}{\partial t} dt \\ =& \left(d\mathbf{r} \cdot \nabla + dt \frac{\partial}{\partial t} \right) F_i \end{aligned} \tag{2.16}$$

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \mathbf{r} \times m\mathbf{v}, \qquad \mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}$$

$$A \times (B \times C) = B(AC) - C(AB) \qquad \mathbf{r} = r\hat{r}$$

$$\begin{aligned} \mathbf{L} =& m(\mathbf{r} \times (\boldsymbol{\omega} \times \mathbf{r})) \\ =& m[\boldsymbol{\omega}(\mathbf{r} \cdot \mathbf{r}) - \mathbf{r}(\mathbf{r} \cdot \boldsymbol{\omega})] \\ =& m[\boldsymbol{\omega}(r^2 \hat{r} \cdot \hat{r}) - r\hat{r}(r\hat{r} \cdot \omega)] \\ =& mr^2[\boldsymbol{\omega} - \hat{r}(\hat{r} \cdot \mathbf{w})] \end{aligned} \tag{2.17}$$

$$I = mr^2 \qquad \mathbf{L} = I\boldsymbol{\omega} \quad \text{if} \quad \hat{r} \cdot \boldsymbol{\omega} = 0$$

2.10 Orthogonal Matrices

(analogy to $\mathbf{a}_i\mathbf{a}_j = \delta_{ij} = \mathbf{a}_i^T \cdot \mathbf{a}_j$)

$$\mathbf{A}^T \cdot \mathbf{A} = \mathbf{1} \qquad \left(\mathbf{A}^T = \mathbf{A}^{-1}\right)$$

$$\mathbf{A}^T = \mathbf{A}^{-1}, \quad \text{therefore} \quad \mathbf{A}^T \cdot \mathbf{A} = \mathbf{1} = \mathbf{1}^T = (\mathbf{A}^T \cdot \mathbf{A})^T$$

Note $det(A) = \pm 1$ if A is orthogonal. Also: A and B orthogonal, then (AB) orthogonal.

Application: Rotation matrices

$$\mathbf{x}_i' = \sum_j A_{ij}\mathbf{x}_j \qquad \text{or} \qquad |\mathbf{x}_i' >= \sum_j |\mathbf{x}_j \times \mathbf{x}_j|\mathbf{x}_i' >$$

example:

$$\begin{pmatrix} \hat{r} \\ \hat{\theta} \\ \hat{\varphi} \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \\ \cos\theta\cos\varphi & \cos\theta\sin\varphi & -\sin\theta \\ -\sin\varphi & \cos\varphi & 0 \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} \tag{2.18}$$

$$\begin{pmatrix} \hat{r} \\ \hat{\theta} \\ \hat{\varphi} \end{pmatrix} = \mathbf{C} \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} \tag{2.19}$$

$$\begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} = \mathbf{C}^{-1} \begin{pmatrix} \hat{r} \\ \hat{\theta} \\ \hat{\varphi} \end{pmatrix} = \mathbf{C}^T \begin{pmatrix} \hat{r} \\ \hat{\theta} \\ \hat{\varphi} \end{pmatrix} \tag{2.20}$$

since $\mathbf{C}^{-1} = \mathbf{C}^T$ ($\mathbf{C}$ is an orthogonal matrix)

Also Euler angles (we will use later. . .)

2.11 Symmetric/Antisymmetric Matrices

Symmetric means $A_{ij} = A_{ji}$, or $\mathbf{A} = \mathbf{A}^T$
Antisymmetric means $A_{ij} = -A_{ji}$, or $\mathbf{A} = -\mathbf{A}^T$

$$\mathbf{A} = \underbrace{\frac{1}{2}\left(\mathbf{A} + \mathbf{A}^T\right)}_{\text{symmetric}} + \underbrace{\frac{1}{2}\left(\mathbf{A} - \mathbf{A}^T\right)}_{\text{antisymmetric}} \tag{2.21}$$

Note also:

$$\begin{aligned} \left(\mathbf{A}\mathbf{A}^T\right)^T &= \left(\mathbf{A}^T\right)^T \mathbf{A}^T \\ &= \mathbf{A}\mathbf{A}^T \end{aligned}$$

Note: $T_r(AB) = 0$ if A is symmetric and B is antisymmetric. Thus $\mathbf{A}\mathbf{A}^T$ $\mathbf{A}^T\mathbf{A}$ are symmetric, but $\mathbf{A} \cdot \mathbf{A}^T \neq \mathbf{A} \cdot \mathbf{A}^T$

Quiz: If $\mathbf{A}$ is an upper triangular matrix, use the Laplacian expansion to determine a formula for $det(A)$ in terms of the elements of A.

2.12 Similarity Transformation

$$\mathbf{A}' = \mathbf{B}\mathbf{A}\mathbf{B}' \tag{2.22}$$

if $\mathbf{B}^{-1} = \mathbf{B}^T$ ($\mathbf{B}$ orthogonal) $\mathbf{B}\mathbf{A}\mathbf{B}^T$ = orthogonal similarity transformation.

2.13 Hermitian (self-adjoint) Matrices

Note:

$$(\mathbf{AB})^* = \mathbf{A}^*\mathbf{B}^*$$
$$(\mathbf{AB})^+ = \mathbf{B}^+\mathbf{A}^+ \quad \text{also} \quad (\mathbf{A}^+)^+ = A$$
$$\mathbf{H}^+ = \mathbf{H} \quad \text{where} \quad \mathbf{H}^+ \equiv (\mathbf{H}^*)^T = (\mathbf{H}^T)^*$$

A real symmetric matrix is Hermitian or a real Hermitian matrix is symmetric (if a matrix is real, Hermitian=symmetric)

2.14 Unitary Matrix

$$\mathbf{U}^+ = \mathbf{U}^{-1}$$

A real orthogonal matrix is unitary or a real unitary matrix is orthogonal (if a matrix is real, unitary=orthogonal)

2.15 Comments about Hermitian Matrices and Unitary Tranformations

1. Unitary tranformations are "norm preserving"

$$\mathbf{x}' = \mathbf{U}\mathbf{x} \qquad (\mathbf{x}')^+\mathbf{x}' = \mathbf{x}^+\mathbf{U}^+\mathbf{U}\mathbf{x} = \mathbf{x}^+ \cdot \mathbf{x}$$

2. More generally, $\mathbf{x}' = \mathbf{U}\mathbf{x}$, $\mathbf{A}' = \mathbf{U}\mathbf{A}\mathbf{U}^+$

$$\mathbf{A}'\mathbf{x}' = \mathbf{U}\mathbf{A}\mathbf{U}^+\mathbf{U}\mathbf{x} = \mathbf{U}(\mathbf{A}\mathbf{x}) \quad \text{and} \quad (\mathbf{y})^+ \cdot \mathbf{A}' \cdot \mathbf{x}' = \mathbf{y}^+\mathbf{U}^+\mathbf{U}\mathbf{A}\mathbf{U}^+\mathbf{U}\mathbf{x}$$

   operation in transformation coordinates = transformation in uniform coordinates = $\mathbf{y}^+\mathbf{A}\mathbf{x}$ (invariant)

3. If $\mathbf{A}^+ = \mathbf{A}$, then $(\mathbf{A}\mathbf{y})^+ \cdot \mathbf{x} = \mathbf{y}^+ \cdot \mathbf{x} = \mathbf{y}^+ \cdot \mathbf{A}^+ \cdot \mathbf{x} = \mathbf{y}^+ \cdot \mathbf{A} \cdot \mathbf{x}$ (Hermitian property)
4. If $\mathbf{A}^+ = \mathbf{A}$, then $(\mathbf{A}')^+ = (\mathbf{U}\mathbf{A}\mathbf{U}^+)^+ = \mathbf{U}\mathbf{A}\mathbf{U}^+$, or $(\mathbf{A}')^+ = \mathbf{A}'$

2.16 More on Hermitian Matrices

$$\mathbf{C} = \frac{1}{2}\underbrace{(\mathbf{C}+\mathbf{C}^+)}_{\text{Hermitian}} + \frac{1}{2}\underbrace{(\mathbf{C}-\mathbf{C}^+)}_{\text{anti-Hermitian}} = \frac{1}{2}(\mathbf{C}+\mathbf{C}^+) + \frac{1}{2i}\cdot\underbrace{i(\mathbf{C}-\mathbf{C}^+)}_{\text{Hermitian!}}$$

Note: $\mathbf{C} = -i[\mathbf{A},\mathbf{B}]$ is Hermitian even if $\mathbf{A}$ and $\mathbf{B}$ are not, (or $i\mathbf{C} = [\mathbf{A},\mathbf{B}]$). $\mathbf{C} = \mathbf{AB}$ is Hermition if $\mathbf{A} = \mathbf{A}^+$, $\mathbf{B} = \mathbf{B}^+$, and $[\mathbf{A},\mathbf{B}] = 0$. A consequence of this is that $\mathbf{C}^n$ is Hermitian if $\mathbf{C}$ is Hermitian. Also, $\mathbf{C} = e^{\alpha\mathbf{A}}$ is Hermitian if $\mathbf{A} = \mathbf{A}^+$, but $\mathbf{C} = e^{i\alpha\mathbf{A}}$ is <u>not</u> Hermitian ($\mathbf{C}$ is unitary). A unitary matrix in general is <u>not</u> Hermitian.

$$f(\mathbf{A}) = \sum_k C_k\mathbf{A}^k \qquad \text{is Hermitian if } C_k \text{ are real}$$

2.17 Eigenvectors and Eigenvalues

Solve $\mathbf{A}\mathbf{c} = a\mathbf{c}$, $(\mathbf{A} - a\mathbf{1})\mathbf{c} = 0$ $det() = 0$ secular equation.

$$\mathbf{A}'\mathbf{c}'_i = a_i\mathbf{c}'_i \qquad \text{Eigenvalue problem}$$

$$\mathbf{A}\mathbf{c}_i = \lambda_i\mathbf{B}\mathbf{c}_i \qquad \text{Generalized eigenvalue problem}$$

$$\mathbf{A}\mathbf{c} = \mathbf{B}\mathbf{c}\boldsymbol{\lambda}$$

If $\mathbf{c}_i^+ \cdot \mathbf{B} \cdot \mathbf{c}_j = \delta_{ij}$ then $\mathbf{c}_i^+ \cdot \mathbf{A} \cdot \mathbf{c}_j = \lambda_i\delta_{ij}$

relation: $\mathbf{A}' = \mathbf{B}^{-\frac{1}{2}}\mathbf{A}\mathbf{B}^{-\frac{1}{2}}$ and $\mathbf{c}'_i = \mathbf{B}^{\frac{1}{2}}\mathbf{c}_i$ (Can always transform. . .Lowden) Example: Hartree-Fock/Kohn-Shon Equations:

$$\mathbf{F}\mathbf{C} = \mathbf{S}\mathbf{C}\boldsymbol{\epsilon}, \quad \mathbf{H}_{eff}\mathbf{C} = \mathbf{S}\mathbf{C}\boldsymbol{\epsilon}$$

For $\mathbf{A}\mathbf{c}_i = \alpha_i\mathbf{c}_i$ if $\mathbf{A} = \mathbf{A}^+ \quad a_i = a_i^*, \quad \mathbf{c}_i^+ \cdot \mathbf{c}_j = \delta_{ij} \qquad \star$ can be chosen

$\mathbf{c}_i$ form a “complete set”

If $\mathbf{A}^+\mathbf{A} = \mathbf{1}, \quad a_i = \pm 1, \quad \mathbf{c}_i^+ \cdot \mathbf{c}_j = \delta_{ij} \qquad \det(A) = \pm 1$

$$\mathbf{H}\mathbf{c}_i = \epsilon_i\mathbf{c}_i \qquad \text{or} \qquad \mathbf{H}\mathbf{c} = \mathbf{c}\boldsymbol{\epsilon}$$

$$\mathbf{c} = \begin{pmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \mathbf{c}_3 \\ \vdots & \vdots & \vdots \end{pmatrix} \tag{2.23}$$

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 & & 0 \\ & \ddots & \\ 0 & & \epsilon_N \end{pmatrix} \tag{2.24}$$

since $\mathbf{c}_i^+ \cdot \mathbf{c}_j = \delta_{ij}, \qquad \mathbf{c}^+ \cdot \mathbf{c} = \mathbf{1}$ and also $\mathbf{c}^+ \cdot \mathbf{H} \cdot \mathbf{c} = \mathbf{c}^+\mathbf{c} = \mathbf{c}^+\mathbf{c}\boldsymbol{\epsilon} = \boldsymbol{\epsilon}$ hence $\mathbf{c}$ is a unitary matrix and is the unitary matrix that diagonalizes $\mathbf{H}$. $\qquad \mathbf{c}^+\mathbf{H}\mathbf{c} = \boldsymbol{\epsilon}$ (eigenvalue spectrum).

2.18 Anti-Hermitian Matrices

Read about them. . .

2.19 Functions of Matrices

$$\mathbf{U}\mathbf{A}\mathbf{U}^+ = \mathbf{a} \qquad \mathbf{A} = \mathbf{U}^+\mathbf{a}\mathbf{U} \quad \text{or} \quad \mathbf{A}\mathbf{U}^+ = \mathbf{U}^+\mathbf{a}$$

$$f(\mathbf{A}) = \mathbf{U}^+ \begin{pmatrix} f(a_1) & & \\ & \ddots & \\ & & f(a_n) \end{pmatrix} \mathbf{U}$$

Power series e.g.

$$e^{\mathbf{A}} = \sum_{k=0}^{\infty} \frac{1}{k!}\mathbf{A}^k$$
$$\sin(\mathbf{A}) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!}\mathbf{A}^{2k+1}$$
$$\cos(\mathbf{A}) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!}\mathbf{A}^{2k}$$

Note:

$$\begin{aligned}\mathbf{A}^2\mathbf{U}^+ =& \mathbf{A}\mathbf{U}\mathbf{U}^+ \\ =& \mathbf{A}\mathbf{U}^+\mathbf{Q} \\ =& \mathbf{U}^+\mathbf{Q}\mathbf{Q} \\ =& \mathbf{U}^+\mathbf{Q}^2\end{aligned}$$

$$\mathbf{Q}^2 \Rightarrow \begin{pmatrix} Q_{11}^2 & 0 \\ 0 & \ddots \end{pmatrix}$$
$$\mathbf{A}^k \cdot \mathbf{U}^+ = \mathbf{U}^+\mathbf{Q}^K$$

Note, if $f(\mathbf{A}) = \sum_k C_k \mathbf{A}^k$ and $\mathbf{U}\mathbf{A}\mathbf{U}^+ = \mathbf{Q}$, then

$$\begin{aligned}\mathbf{F} =& f(\mathbf{A})\mathbf{U}^+ \\ =& \sum_k c_k \mathbf{U}^+\mathbf{Q}^k \\ =& \mathbf{U}^+ \sum_k c_k \mathbf{Q}^k \\ =& \mathbf{U}^+ \begin{pmatrix} f(a_{11}) & & \\ & \ddots & \\ & & f(a_{nn}) \end{pmatrix} = \mathbf{U}^+\mathbf{f}\end{aligned} \tag{2.25}$$

so if $\mathbf{U}\mathbf{A}\mathbf{U}^+ = \mathbf{Q}$, then $\mathbf{U}\mathbf{F}\mathbf{U}^+ = \mathbf{f}$ and $f_{ij} = f(a_i)\delta_{ij}$
Also:
Trace Formula

$$det(e^{\mathbf{A}}) = e^{Tr(A)} \qquad \text{(special case of} \quad det[f(\mathbf{A})] = \pi_i f(a_{ii}))$$

Baker-Hausdorff Formula

$$e^{i\mathbf{G}}\mathbf{H}e^{-i\mathbf{G}} = \mathbf{H} + [i\mathbf{G}\mathbf{H}] + \frac{1}{2}[i\mathbf{G}, [i\mathbf{G}, \mathbf{H}]] + \cdots$$

Note, if

$$\mathbf{A}\mathbf{U}^+ = \mathbf{U}^+\mathbf{Q}\mathbf{A}(\lambda) = \mathbf{A} + \lambda\mathbf{1}$$

so has some eigenvectors, but eigenvalues are shifted.

$$\mathbf{A}(\lambda)\mathbf{U}^+ = (\mathbf{A} + \lambda\mathbf{1})\mathbf{U}^+ = \mathbf{U}^+\mathbf{Q} + \mathbf{U}^+\lambda\mathbf{1} = \mathbf{U}^+(\mathbf{Q} + \lambda\mathbf{1}) = \mathbf{U}^+\mathbf{Q}(\lambda)$$

2.20 Normal Marices

$$[\mathbf{A}, \mathbf{A}^{+}] = 0 \qquad \text{(Hermitian and real symmetry are specific cases)}$$

$$\mathbf{A}\mathbf{c}_i = a_i \mathbf{c}_i, \quad \mathbf{A}^{+}\mathbf{c}_i = a_i^{*} \mathbf{c}_i, \quad \mathbf{c}_i^{+} \cdot \mathbf{c}_j = 0$$

2.21 Matrix

2.21.1 Real Symmetric

$$\mathbf{A} = \mathbf{A}^{T} = \mathbf{A}^{+} \qquad a_i \text{ real} \qquad \mathbf{c}_i^{T} \cdot \mathbf{c}_j = \delta_{ij} \qquad \text{Hermitian normal}$$

2.21.2 Hermitian

$$\mathbf{A} = \mathbf{A}^{+} \qquad a_i \text{ real} \qquad \mathbf{c}_i^{+} \cdot \mathbf{c}_j = \delta_{ij} \qquad \text{normal}$$

2.21.3 Normal

$$[\mathbf{A}, \mathbf{A}^{+}] = 0 \qquad \text{if } \mathbf{A}\mathbf{c}_i = a_i \mathbf{c}_i \qquad \mathbf{c}_i^{+} \cdot \mathbf{c}_j = \delta_{ij}$$

2.21.4 Orthogonal

$$\mathbf{U}^{T} \cdot \mathbf{U} = 1 \quad (\mathbf{U}^{T} = \mathbf{U}^{-1}) \qquad a_i\,(\pm 1) \qquad \mathbf{c}_i^{T} \cdot \mathbf{c}_j = \delta_{ij} \qquad \text{unitary, normal}$$

2.21.5 Unitary

$$\mathbf{U}^{+}\mathbf{U} = 1 \quad (\mathbf{U}^{+} = \mathbf{U}^{-1}) \qquad a_i \text{ real}\,(\pm 1) \qquad \mathbf{c}_i^{+} \cdot \mathbf{c}_j = \delta_{ij} \qquad \text{normal}$$

If $\mathbf{U}\mathbf{A}\mathbf{U}^{+} = \mathbf{a}$, and $\mathbf{U}^{+}\mathbf{U} = \mathbf{1}$ then $[\mathbf{A}, \mathbf{A}^{+}] = 0$ and conversely.

Chapter 3

Calculus of Variations

3.1 Functions and Functionals

Here we consider *functions* and *functionals* of a single argument (a variable and function, respectively) in order to introduce the extension of the conventional function calculus to that of functional calculus.

- A **function** $f(x)$ is a prescription for transforming a numerical argument x into a number; e.g. $f(x) = 1 + x^2 + e^{-x}$.
- A **functional** $F[y]$ is a prescription for transforming a function argument $y(x)$ into a number; e.g. $F[y] = \int_{x_1}^{x_2} y^2(x) \cdot e^{-sx}\, dx$.

Hence, a functional requires knowledge of it's function argument (say $y(x)$) not at a single numerical point x, in general, but rather over the entire domain of the function's numerical argument x (i.e., over all x in the case of $y(x)$). Alternately stated, a functional is often written as some sort of integral (see below) where the argument of y (we have been referring to it as "x") is a dummy integration index that gets integrated out.

In general, a functional $F[y]$ of the 1-dimensional function $y(x)$ may be written

$$F[y] = \int_{x_1}^{x_2} f\left(x, y(x), y'(x), \cdots y^{(n)}(x), \right)\, dx \tag{3.1}$$

where f is a (multidimensional) function, and $y' \equiv dy/dx\,, \cdots\; y^n \equiv d^n y/dx^n$. For the purposes here, we will consider the bounday conditions of the function argument y are such that $y, y' \cdots y^{(n-1)}$ **have fixed values at the endpoints**; i.e.,

$$y^{(j)}(x_1) = y_1^{(j)}\,, \quad y^{(j)}(x_2) = y_2^{(j)} \quad \text{for } j = 0, \cdots (n-1) \tag{3.2}$$

where $y_1^{(j)}$ and $y_2^{(j)}$ are constants, and $y^{(0)} \equiv y$.

In standard function calculus, the derivative of a function $f(x)$ with respect to x is defined as the limiting process

$$\left[\frac{df}{dx}\right]_x \equiv \lim_{\epsilon\to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon} \tag{3.3}$$

(read "the derivative of f with respect to x, evaluated at x). The *function derivative* indicates how $f(x)$ changes when x changes by an infintesimal amount from x to $x + \epsilon$.

Analogously, we define the functional derivative of $F[y]$ with respect to the function y *at a particular point* x_0 by

$$\left[\frac{\delta F}{\delta y(x)}\right]_{y(x_0)} \equiv \lim_{\epsilon\to 0} \frac{F[y + \epsilon\delta(x - x_0)] - F[y]}{\epsilon} \tag{3.4}$$

(read, "the functional derivative of F with respect to y, evaluated at the point $y(x_0)$). This *functional derivative* indicates how $F[y]$ changes when the function $y(x)$ is changed by an infintesimal amount at the point $x = x_0$ from $y(x)$ to $y(x) + \epsilon\delta(x - x_0)$.

We now procede formally to derive these relations.

3.2 Functional Derivatives: Formal Development in 1-Dimension

Consider the problem of finding a *function* $y(x)$ that corresponds to a stationary condition (an extremum value) of the functional $F[y]$ of Eq. 3.1, subject to the boundary conditions of Eq. 3.2; i.e., that the function y and a sufficient number of it's derivatives are fixed at the boundary. For the purposes of describing variations, we define the function

$$y(x,\epsilon) \quad = \quad y(x) + \epsilon\eta(x) = y(x,0) + \epsilon\eta(x) \tag{3.5}$$

where $\eta(x)$ is an arbitrary differentiable function that satisfies the end conditions $\eta^{(j)}(x_1) = \eta^{(j)}(x_2) = 0$ for $j = 1, \cdots (n-1)$ such that in any variation, the boundary conditions of Eq. 3.2 are preserved; i.e., that $y^{(j)}(x_1) = y_1^{(j)}$ and $y^{(j)}(x_2) = y_2^{(j)}$ for $j = 0, \cdots (n-1)$. It follows the derivative relations

$$y^{(j)}(x,\epsilon) \quad = \quad y^{(j)}(x) + \epsilon\eta^{(j)}(x) \tag{3.6}$$

$$\frac{d}{d\epsilon}y^{(j)}(x,\epsilon) \quad = \quad \eta^{(j)}(x) \tag{3.7}$$

where superscript j ($j = 0, \cdots n$) in parentheses indicates the order of the derivative with respect to x. To remind, here n is the highest order derivative of y that enters the functional $F[y]$. For many examples in physics $n = 1$ (such as we will see in classical mechanics), and only the *fixed end points* of y itself are required; however, in electrostatics and quantum mechanics often higher order derivatives are involved, so we consider the more general case.

If $y(x)$ is the function that corresponds to an extremum of $F[y]$, we expect that *any* infintesimal variation $\epsilon\eta(x)$ away from y that is sufficiently smooth and subject to the fixed-endpoint boundary conditions of Eq. 3.2) will have zero effect (to first order) on the extremal value. The "arbitrary" function $\eta(x)$ of course has been defined to satisfy the differentiability and boundary conditions, and the scale factor ϵ allows a mechanism for effecting infintesimal variations through a limiting procedure approaching $\epsilon = 0$. At $\epsilon = 0$, the varied function $y(x,\epsilon)$ is the extremal value $y(x)$. Mathematically, this implies

$$\begin{aligned}
\frac{d}{d\epsilon}\left[F[y+\epsilon\eta]\right]_{\epsilon=0} \quad &= \quad 0 \\
&= \quad \frac{d}{d\epsilon}\left[\int_{x_1}^{x_2} f(x, y(x,\epsilon), y'(x,\epsilon), \cdots)\, dx\right]_{\epsilon=0} \\
&= \quad \int_{x_1}^{x_2} \left\{ \left(\frac{\partial f}{\partial y}\right)\frac{\partial y(x,\epsilon)}{\partial\epsilon} + \left(\frac{\partial f}{\partial y'}\right)\frac{\partial y'(x,\epsilon)}{\partial\epsilon} + \cdots \right\} dx \\
&= \quad \int_{x_1}^{x_2} \left\{ \left(\frac{\partial f}{\partial y}\right)\eta(x) + \left(\frac{\partial f}{\partial y'}\right)\eta'(x) + \cdots \right\} dx
\end{aligned} \tag{3.8}$$

where we have used $\partial y(x,\epsilon)/\partial\epsilon = \eta(x)$, $\partial y'(x,\epsilon)/\partial\epsilon = \eta'(x)$, etc... If we integrate by parts the term in Eq. 3.8 involving $\eta'(x)$ we obtain

$$\begin{aligned}
\int_{x_1}^{x_2}\left(\frac{\partial f}{\partial y'}\right)\eta'(x)\, dx \quad &= \quad \left(\frac{\partial f}{\partial y'}\right)\eta(x)\Bigg|_{x_1}^{x_2} - \int_{x_1}^{x_2}\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right)\eta(x)\, dx \\
&= \quad -\int_{x_1}^{x_2}\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right)\eta(x)\, dx
\end{aligned} \tag{3.9}$$

where we have used the fact that $\eta(x_1) = \eta(x_2) = 0$ to cause the boundary term to vanish. More generally, for all the derivative terms in Eq. 3.8 we obtain

$$\int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y^{(j)}}\right) \eta^{(j)}(x)\, dx \quad = \quad (-1)^{(j)} \int_{x_1}^{x_2} \frac{d^j}{dx^j} \left(\frac{\partial f}{\partial y^{(j)}}\right) \eta(x)\, dx \tag{3.10}$$

for $j = 1, \cdots n$ where we have used the fact that $\eta^{(j)}(x_1) = \eta^{(j)}(x_2) = 0$ for $j = 0, \cdots (n-1)$ to cause the boundary terms to vanish. Substituting Eq. 3.10 in Eq. 3.8 gives

$$\begin{aligned} \frac{d}{d\epsilon} \left[F[y + \epsilon\eta]\right]_{\epsilon=0} &= \int_{x_1}^{x_2} \left\{ \left(\frac{\partial f}{\partial y}\right) - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) + \cdots \right. \\ &\quad \left. + (-1)^n \frac{d^n}{dx^n}\left(\frac{\partial f}{\partial y^{(n)}}\right) \right\} \eta(x)\, dx \\ &= 0 \end{aligned} \tag{3.11}$$

Since $\eta(x)$ is an arbitrary differential function subject to the boundary conditions of Eq. 3.2, the terms in brackets must vanish. This leads to a generalized form of the Euler equation in one dimension for the extremal value of $F[y]$ of Eq. 3.4

$$\left(\frac{\partial f}{\partial y}\right) - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) + \cdots + (-1)^n \frac{d^n}{dx^n}\left(\frac{\partial f}{\partial y^{(n)}}\right) = 0 \tag{3.12}$$

In other words, for the function $y(x)$ to correspond to an extremal value of $F[y]$, Eq. 3.12 must be satisfied for *all* $y(x)$; i.e., over the entire domain of x of $y(x)$. Consequently, solution of Eq. 3.12 requires solving for an entire *function* - not just a particular value of the function argument x as in function calculus. Eq. 3.12 is referred to as the Euler equation (1-dimensional, in this case), and typically results in a differential equation, the solution of which (subject to the boundary conditions already discussed) provides the function $y(x)$ that produces the extremal value of the functional $F[y]$.

We next define a more condensed notation, and derive several useful techniques such as algebraic manipulation of functionals, functional derivatives, chain relations and Taylor expansions. We also explicitly link the functional calculus back to the traditional function calculus in certain limits.

3.3 Variational Notation

We define $\delta F[y]$, the "variation of the functional $F[y]$", as

$$\begin{aligned} \delta F[y] &\equiv \frac{d}{d\epsilon}\left[F[y+\epsilon\eta]\right]_{\epsilon=0} \epsilon \\ &= \int_{x_1}^{x_2} \left\{ \left(\frac{\partial f}{\partial y}\right) - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) + \cdots + (-1)^n \frac{d^n}{dx^n}\left(\frac{\partial f}{\partial y^{(n)}}\right) \right\} \eta(x)\epsilon\, dx \\ &= \int_{x_1}^{x_2} \frac{\delta F}{\delta y(x)} \delta y(x)\, dx \end{aligned} \tag{3.13}$$

where (analagously) $\delta y(x)$, the "variation of the function $y(x)$", is defined by

$$\begin{aligned} \delta y(x) &\equiv \frac{d}{d\epsilon}\left[y(x) + \epsilon\eta(x)\right]_{\epsilon=0} \epsilon \\ &= \epsilon\eta(x) \\ &= y(x,\epsilon) - y(x,0) \end{aligned} \tag{3.14}$$

where we have again used the identity $y(x,0) = y(x)$. Relating the notation of the preceding section, we have

$$y(x,\epsilon) = y(x) + \epsilon\eta(x) = y(x) + \delta y(x) \tag{3.15}$$

Note that the operators δ and d/dx commute; i.e., that $\delta(d/dx) = (d/dx)\delta$:

$$\begin{aligned}\delta y'(x) &= \delta\frac{dy}{dx} = \frac{d}{d\epsilon}\left[\frac{d}{dx}\left(y+\epsilon\eta\right)\right]_{\epsilon=0}\epsilon \\ &= \frac{d}{d\epsilon}\left[\left(y'+\epsilon\eta'\right)\right]_{\epsilon=0}\epsilon = \eta'\epsilon = \frac{d}{dx}\left(\eta\epsilon\right) = \frac{d}{dx}\delta y\end{aligned} \tag{3.16}$$

Hence the (first) functional variation of $F[y]$ can be written

$$\delta F[y] = \int_{x_1}^{x_2} \frac{\delta F}{\delta y(x)}\delta y(x)\,dx \tag{3.17}$$

where $\frac{\delta F}{\delta y(x)}$ is defined as "the (first) functional derivative of $F[y]$ with respect to y at position x", and assuming $F[y]$ in the form of Eq. 3.1, is given by

$$\frac{\delta F}{\delta y(x)} = \left(\frac{\partial f}{\partial y}\right) - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) + \cdots + (-1)^n\frac{d^n}{dx^n}\left(\frac{\partial f}{\partial y^{(n)}}\right) \tag{3.18}$$

Note that the functional derivative defined above is itself a function of x. In fact, Eq. 3.17 can be considered as a generalization of an exact differential of a discreet multivariable function in calculus, .e.g.,

$$dF(x_1, x_2, \cdots, x_N) = \sum_i \frac{\partial F}{\partial x_i}dx_i \tag{3.19}$$

where the summation over discreet variables x_i has been replaced by integration over a continuous set of variables x.

An extremal value of $F[y]$ is a solution of the stationary condition

$$\delta F[y] = 0 \tag{3.20}$$

and can be found by solution of the Euler equation 3.12.

3.4 Functional Derivatives: Elaboration

3.4.1 Algebraic Manipulations of Functional Derivatives

The functional derivative has properties analogous to a normal function derivative

$$\frac{\delta}{\delta y(x)}\left(c_1F_1 + c_2F_2\right) = c_1\frac{\delta F_1}{\delta y(x)} + c_2\frac{\delta F_2}{\delta y(x)} \tag{3.21}$$

$$\frac{\delta}{\delta y(x)}\left(F_1F_2\right) = \frac{\delta F_1}{\delta y(x)}F_2 + F_1\frac{\delta F_2}{\delta y(x)} \tag{3.22}$$

$$\frac{\delta}{\delta y(x)}\left(\frac{F_1}{F_2}\right) = \left(\frac{\delta F_1}{\delta y(x)}F_2 - F_1\frac{\delta F_2}{\delta y(x)}\right)/F_2^2 \tag{3.23}$$

3.4.2 Generalization to Functionals of Higher Dimension

The expression for the functional derivative in Eq. 3.18 can be generalized to multidimensional functions in a straight forward manner.

$$\frac{\delta F}{\delta\rho(x_1,\cdots x_N)} = \left(\frac{\partial f}{\partial \rho}\right) + \sum_{j=1}^{n}(-1)^j \sum_{i=1}^{N} \frac{\partial^j}{\partial x_i^j}\left(\frac{\partial f}{\partial \rho_{x_i}^{(j)}}\right) \tag{3.24}$$

The functional derivative in the 3-dimensional case is

$$\frac{\delta F}{\delta\rho(\mathbf{r})} = \left(\frac{\partial f}{\partial \rho}\right) - \nabla\cdot\left(\frac{\partial f}{\partial \nabla\rho}\right) + \nabla^2\left(\frac{\partial f}{\partial \nabla^2\rho}\right) - \cdots \tag{3.25}$$

Example: Variational principle for a 1-particle quantum system.

Consider the energy of a 1-particle system in quantum mechanics subject to an external potential $v(\mathbf{r})$. The system is described by the 1-particle Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \tag{3.26}$$

The expectation value of the energy given a trial wave function $\tilde{\Psi}(\mathbf{r})$ is given by

$$\begin{aligned} E[\tilde{\Psi}] &= \frac{\int \tilde{\Psi}^*(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right)\tilde{\Psi}(\mathbf{r})d^3r}{\int \tilde{\Psi}^*(\mathbf{r})\tilde{\Psi}(\mathbf{r})d^3r} \\ &= \frac{\left\langle \tilde{\Psi}\left|\hat{H}\right|\tilde{\Psi}\right\rangle}{\langle\tilde{\Psi}|\tilde{\Psi}\rangle} \end{aligned} \tag{3.27}$$

Let us see what equation results when we require that the energy is an extremal value with respect to the wave function; i.e.,

$$\frac{\delta E[\Psi]}{\delta\Psi(\mathbf{r})} = 0 \tag{3.28}$$

Where we denote the wave function that produces this extremal value Ψ. Since this is a 1-particle system in the absence of magnetic fields, there is no need to consider spin explicitly or to enforce antisymmetry of the wave function as we would in a many-particle system. Moreover, there is no loss of generality if we restrict the wave function to be real (one can double the effort in this example by considering the complex case, but the manipulations are redundant, and it does not add to the instructive value of the variational technique - and a student's time is valuable!). Finally, note that we have constructed the energy functional $E[\tilde{\Psi}]$ to take on an un-normalized wave function and return a correct energy (that is to say, the normalization is built into the energy expression), alleviating the need to explicitly constrain the wave function to be normalized in the variational process. We return to this point in a later example using the method of Lagrange multipliers.

Recall from Eq. 3.23 we have

$$\frac{\delta E[\Psi]}{\delta\Psi(\mathbf{r})} = \left(\frac{\delta\left\langle\Psi\left|\hat{H}\right|\Psi\right\rangle}{\delta\Psi(\mathbf{r})}\langle\Psi|\Psi\rangle - \frac{\delta\langle\Psi|\Psi\rangle}{\delta\Psi(\mathbf{r})}\left\langle\Psi\left|\hat{H}\right|\Psi\right\rangle\right)/\langle\Psi|\Psi\rangle^2 \tag{3.29}$$

Let us consider in more detail the first functional derivative term,

$$\frac{\delta\left\langle\Psi\left|\hat{H}\right|\Psi\right\rangle}{\delta\Psi(\mathbf{r})} = \frac{\delta}{\delta\Psi(\mathbf{r})}\int\tilde{\Psi}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right)\tilde{\Psi}(\mathbf{r})d^3r \tag{3.30}$$

where we have dropped the complex conjugation since we consider the case where Ψ is real. It is clear that the integrand, as written above, depends explicitly only on Ψ and $\nabla^2\Psi$. Using Eq. 3.25 (the specific 3-dimensional case of Eq. 3.24), we have that

$$\begin{aligned} \frac{\partial f}{\partial \Psi(\mathbf{r})} &= \frac{-\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + 2v(\mathbf{r})\Psi(\mathbf{r}) \\ \left(\frac{\partial f}{\partial \nabla^2\Psi(\mathbf{r})}\right) &= \left(\frac{-\hbar^2}{2m}\Psi(\mathbf{r})\right) \end{aligned} \tag{3.31}$$

and thus

$$\frac{\delta\left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle}{\delta\Psi(\mathbf{r})} = 2\left(\frac{-\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\right)\Psi(\mathbf{r}) = 2\hat{H}\Psi(\mathbf{r}) = 2\hat{H}|\Psi\rangle \tag{3.32}$$

where the last equality simply reverts back to Bra-Ket notation. Similarly, we have that

$$\frac{\delta\langle\Psi|\Psi\rangle}{\delta\Psi(\mathbf{r})} = 2\Psi(\mathbf{r}) = 2|\Psi\rangle \tag{3.33}$$

This gives the Euler equation

$$\begin{aligned} \frac{\delta E[\Psi]}{\delta\Psi(\mathbf{r})} &= \left(2\hat{H}|\Psi\rangle\langle\Psi|\Psi\rangle - 2|\Psi\rangle\left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle\right)/\langle\Psi|\Psi\rangle^2 \\ &= 2\left(\frac{\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{|\Psi\rangle\left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle}{\langle\Psi|\Psi\rangle^2}\right) \\ &= 0 \end{aligned} \tag{3.34}$$

Multiplying through by $\langle\Psi|\Psi\rangle$, dividing by 2 and substituting in the expression for $E[\Psi]$ above we obtain

$$\hat{H}|\Psi\rangle = \frac{\left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle}{\langle\Psi|\Psi\rangle}|\Psi\rangle = E[\Psi]|\Psi\rangle \tag{3.35}$$

which is, of course, just the stationary-state Schrödinger equation.

3.4.3 Higher Order Functional Variations and Derivatives

Higher order functional variations and functional derivatives follow in a straight forward manner from the corresponding first order definitions. The second order variation is $\delta^2 F = \delta(\delta F)$, and similarly for higher order variations. Second and higher order functional derivatives are defined in an analogous way.

The solutions of the Euler equations are *extremals* - i.e., stationary points that correspond to maxima, minima or saddle points (of some order). The nature of the stationary point can be discerned (perhaps not completely) by consideration of the second functional variation. For a functional $F[f]$, suppose f_0 is the function that solves the Euler equation; i.e., that satisfies $\delta F[f] = 0$ or equivalently $[\delta F[f]/\delta f(x)]_{f=f_0} = 0$, then

$$\delta^2 F = \frac{1}{2}\int\int \delta f(x)\left[\frac{\delta^2 F}{\delta f(x)\delta f(x')}\right]_{f=f_0}\delta f(x')\,dx\,dx' \tag{3.36}$$

The stationary point of $F[f_0]$ at f_0 can be characterized by

$$\begin{aligned} \delta^2 F \geq 0 &\quad : \quad \text{minimum} \\ \delta^2 F = 0 &\quad : \quad \text{saddle point (order undetermined)} \\ \delta^2 F \leq 0 &\quad : \quad \text{maximum} \end{aligned} \tag{3.37}$$

Example: Second functional derivatives.

Consider the functional for the classical electrostatic energy

$$J[\rho] = \frac{1}{2}\int\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r d^3r' \tag{3.38}$$

what is the second functional derivative $\left[\frac{\delta^2 J[\rho]}{\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')}\right]$?

The first functional derivative with respect to $\rho(\mathbf{r})$ is

$$\begin{aligned} \frac{\delta J[\rho]}{\delta\rho(\mathbf{r})} &= \frac{1}{2}\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r' + \frac{1}{2}\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r' \\ &= \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r' \end{aligned} \tag{3.39}$$

Note, $\mathbf{r}'$ is merely a dummy integration index - it could have been called $\mathbf{x}$, $\mathbf{y}$, $\mathbf{r}'''$, etc... The important feature is that after integration what results is a function of $\mathbf{r}$ - the same $\mathbf{r}$ that is indicated by the functional derivative $\frac{\delta J[\rho]}{\delta\rho(\mathbf{r})}$.

The second functional derivative with respect to $\rho(\mathbf{r}')$ is

$$\begin{aligned} \left[\frac{\delta^2 J[\rho]}{\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')}\right] &= \frac{\delta}{\delta\rho(\mathbf{r}')}\frac{\delta J[\rho]}{\delta\rho(\mathbf{r})} \\ &= \frac{\delta}{\delta\rho(\mathbf{r}')}\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r' \\ &= \frac{1}{|\mathbf{r}-\mathbf{r}'|} \end{aligned} \tag{3.40}$$

3.4.4 Integral Taylor series expansions

An integral Taylor expansion for $F[f_0 + \Delta f]$ is defined as

$$\begin{aligned} F[f_0+\Delta f] &= F[f_0] \\ &+ \sum_{n=1}^{\infty}\frac{1}{n!}\int\int\cdots\int\left[\frac{\delta^{(n)}F}{\delta f(x_1)\delta f(x_2)\cdots\delta f(x_n)}\right]_{f_0} \\ &\times\Delta f(x_1)\Delta f(x_2)\cdots\Delta f(x_n)\, dx_1 dx_2\cdots dx_n \end{aligned} \tag{3.41}$$

For functionals of more than one function, e.g. $F[f,g]$, mixed derivatives can be defined. Typically, for sufficiently well behaved functionals, the order of the functional derivative operations is not important (i.e., they commute),

$$\frac{\delta^2 F}{\delta f(x)\delta g(x')} = \frac{\delta^2 F}{\delta g(x)\delta f(x')} \tag{3.42}$$

An integral Taylor expansion for $F[f_0 + \Delta f, g_0 + \Delta g]$ is defined as

$$\begin{aligned} F[f_0 + \Delta f, g_0 + \Delta g] &= F[f_0, g_0] \\ &+ \int \left[\frac{\delta F}{\delta f(x)}\right]_{f_0,g_0} \Delta f(x)\, dx \\ &+ \int \left[\frac{\delta F}{\delta g(x)}\right]_{f_0,g_0} \Delta g(x)\, dx \\ &+ \frac{1}{2}\int\int \Delta f(x) \left[\frac{\delta^2 F}{\delta f(x)\delta f(x')}\right]_{f_0,g_0} \Delta f(x')\, dx dx' \\ &+ \int\int \Delta f(x) \left[\frac{\delta^2 F}{\delta f(x)\delta g(x')}\right]_{f_0,g_0} \Delta g(x')\, dx dx' \\ &+ \frac{1}{2}\int\int \Delta g(x) \left[\frac{\delta^2 F}{\delta g(x)\delta g(x')}\right]_{f_0,g_0} \Delta g(x')\, dx dx' \\ &+ \cdots \end{aligned} \tag{3.43}$$

3.4.5 The chain relations for functional derivatives

From Eq. 3.13, the variation of a functional $F[f]$ is given by

$$\delta F = \int \frac{\delta F}{\delta f(x)} \delta f(x)\, dx \tag{3.44}$$

(where it is understood we have dropped the definite integral notation with endpoinds x_1 and x_2 - it is also valid that the boundaries be at plus or minus infinity). If at each point x, $f(x)$ itself is a functional of another function g, we write $f = f[g(x), x]$ (an example is the electrostatic potential $\phi(\mathbf{r})$ which at every point $\mathbf{r}$ is a functional of the charge density ρ at all points), we have

$$\delta f(x) = \int \frac{\delta f(x)}{\delta g(x')} \delta g(x')\, dx \tag{3.45}$$

which gives the integral chain relation

$$\begin{aligned} \delta F &= \int\int \frac{\delta F}{\delta f(x)} \frac{\delta f(x)}{\delta g(x')} \delta g(x')\, dx dx' \\ &= \int \frac{\delta F}{\delta g(x')} \delta g(x')\, dx' \end{aligned} \tag{3.46}$$

hence,

$$\frac{\delta F}{\delta g(x')} = \int \frac{\delta F}{\delta f(x)} \frac{\delta f(x)}{\delta g(x')}\, dx \tag{3.47}$$

Suppose $F[f]$ is really an ordinary function (a special case of a functional); i.e. $F = F(f)$, then written as a functional

$$F(f(x)) = \int F(f(x'))\delta(x' - x) dx' \tag{3.48}$$

it follows that

$$\frac{\delta F(f(x))}{\delta f(x')} = \frac{dF}{df} \delta(x' - x) \tag{3.49}$$

If we take $F(f) = f$ itself, we see that

$$\frac{\delta f(x)}{\delta f(x')} = \delta(x' - x) \tag{3.50}$$

If instead we have a function that takes a functional argument, e.g. $g = g(F[f(x)])$, then we have

$$\begin{aligned}\frac{\delta g}{\delta f(x)} &= \int \frac{\delta g}{\delta F[f,x']}\frac{\delta F[f,x']}{\delta f(x)}\,dx' \\ &= \int \frac{dg}{dF[f,x']}\delta(x'-x)\frac{\delta F[f,x']}{\delta f(x)}\,dx' \\ &= \frac{dg}{dF}\frac{\delta F}{\delta f(x)} \end{aligned} \tag{3.51}$$

If the argument f of the functional $F[f]$ contains a parameter λ; i.e., $f = f(x;\lambda)$, then the derivative of $F[f]$ with respect to the parameter is given by

$$\frac{\partial F[f(x;\lambda)]}{\partial\lambda} = \int \frac{\delta F}{\delta f(x;\lambda)}\frac{\partial f(x;\lambda)}{\partial\lambda}\,dx \tag{3.52}$$

3.4.6 Functional inverses

For ordinary function derivatives, the inverse is defined as $(dF/df)^{-1} = df/dF$ such that $(dF/df)^{-1}\cdot(df/dF) = 1$, and hence is unique. In the case of functional derivatives, the relation between $F[f]$ and $f(x)$ is in general a reduced dimensional mapping; i.e., the scalar $F[f]$ is determined from many (often an infinite number) values of the function argument $f(x)$.

Suppose we have the case where we have a function $f(x)$, each value of which is itself a functional of another function $g(x')$. Moreover, assume that this relation is invertable; i.e., that each value of $g(x')$ can be written as a functional of $f(x)$. A simple example would be if $f(x)$ were a smooth function, and $g(x')$ was the Fourier transform of $f(x)$ (usually the x' would be called k or ω or something...). For this case we can write

$$\delta f(x) = \int \frac{\delta f(x)}{\delta g(x')}\delta g(x')\,dx' \tag{3.53}$$

$$\delta g(x') = \int \frac{\delta g(x')}{\delta f(x'')}\delta f(x'')\,dx'' \tag{3.54}$$

which leads to

$$\delta f(x) = \int\int \frac{\delta f(x)}{\delta g(x')}\frac{\delta g(x')}{\delta f(x'')}\delta f(x'')\,dx'\,dx'' \tag{3.55}$$

providing the reciprocal relation

$$\int \frac{\delta f(x)}{\delta g(x')}\frac{\delta g(x')}{\delta f(x'')}\,dx' = \frac{\delta f(x)}{\delta f(x'')} = \delta(x-x'') \tag{3.56}$$

We now *define* the inverse as

$$\left[\frac{\delta f(x)}{\delta g(x')}\right]^{-1} = \frac{\delta g(x')}{\delta f(x)} \tag{3.57}$$

from which we obtain

$$\int \frac{\delta f(x)}{\delta g(x')}\left[\frac{\delta f(x)}{\delta g(x')}\right]^{-1}\,dx' = \delta(x-x'') \tag{3.58}$$

3.5 Homogeneity and convexity properties of functionals

In this section we define two important properties, homogeneity and convexity, and discuss some of the powerful consequences and inferences that can be ascribed to functions and functionals that have these properties.

3.5.1 Homogeneity properties of functions and functionals

A function $f(x_1, x_2 \cdots)$ is said to be *homogeneous of degree k* (in all of it's degrees of freedom) if

$$f(\lambda x_1, \lambda x_2, \cdots) \quad = \quad \lambda^k f(x_1, x_2 \cdots) \tag{3.59}$$

and similarly, a functional $F[f]$ is said to be *homogeneous of degree k* if

$$F[\lambda f] \quad = \quad \lambda^k F[f] \tag{3.60}$$

Thus homogeneity is a type of *scaling relationship* between the value of the function or functional with unscaled arguments and the corresponding values with scaled arguments. If we differentiate Eq. 3.59 with respect to λ we obtain for the term on the left-hand side

$$\frac{df(\lambda x_1, \lambda x_2, \cdots)}{d\lambda} \quad = \quad \frac{\partial f(\lambda x_1, \lambda x_2, \cdots)}{\partial(\lambda x_i)} \frac{d(\lambda x_i)}{d\lambda} \tag{3.61}$$

$$= \quad \sum_i x_i \frac{\partial f(\lambda x_1, \lambda x_2, \cdots)}{\partial(\lambda x_i)} \tag{3.62}$$

(where we note that $d(\lambda x_i)/d\lambda = x_i$), and for the term on the right-hand side

$$\frac{d}{d\lambda}\Big(\lambda^k f(x_1, x_2, \cdots)\Big) \quad = \quad k\lambda^{k-1} f(x_1, x_2, \cdots) \tag{3.63}$$

Setting $\lambda = 1$ and equating the left and right-hand sides we obtain the important relation

$$\sum_i x_i \frac{\partial f(x_1, x_2, \cdots)}{\partial x_i} \quad = \quad k f(x_1, x_2, \cdots) \tag{3.64}$$

Similarly, for homogeneous functionals we can derive an analogous relation

$$\int \frac{\delta F}{\delta f(x)} f(x)\, dx \quad = \quad kF[f] \tag{3.65}$$

Sometimes these formulas are referred to as *Euler's theorem for homogeneous functions/functionals*. These relations have the important conseuqnce that, for homogeneous functions (functionals), the value of the function (functional) can be derived from knowledge only of the function (functional) derivative.

For example, in thermodynamics, *extensive* quantities (such as the Energy, Enthalpy, Gibbs free energy, etc...) are homogeneous functionals of degree 1 in their extensive variables (like entropy, volume, the number of particles, etc...). and *intensive* quantities (such as the pressure, etc...) are homogeneous functionals of degree 0. Consider the energy as a function of entropy S, volume V, and particle number n_i for each type of particle (i represents a type of particle). Then we have that $E = E(S, V, n_1, n_2 \cdots)$ and

$$E \quad = \quad E(S, V, n_1, n_2 \cdots) \tag{3.66}$$

$$dE \quad = \quad \left(\frac{\partial E}{\partial S}\right)_{V,n_i} dS + \left(\frac{\partial E}{\partial V}\right)_{S,n_i} dV + \sum_i \left(\frac{\partial E}{\partial n_i}\right)_{S,V,n_{j\neq i}} dn_i \tag{3.67}$$

$$= \quad TdS - pdV + \sum_i \mu_i dn_i$$

where we have used the identities $\left(\frac{\partial E}{\partial S}\right)_{V,n_i} = T$, $\left(\frac{\partial E}{\partial V}\right)_{S,n_i} = -p$, and $\left(\frac{\partial E}{\partial n_i}\right)_{S,V,n_{j\neq i}} = \mu_i$. From the first-order homogeneity of the extensive quantity $E(S, V, n_1, n_2 \cdots)$ we have that

$$E(\lambda S, \lambda V, \lambda n_1, \lambda n_2, \cdots) = \lambda E(S, V, n_1, n_2 \cdots) \tag{3.68}$$

The Euler theorem for first order homogeneous functionals then gives

$$\begin{aligned} E &= \left(\frac{\partial E}{\partial S}\right)_{V,n_i} S + \left(\frac{\partial E}{\partial V}\right)_{S,n_i} V + \sum_i \left(\frac{\partial E}{\partial n_i}\right)_{S,V,n_{j\neq i}} n_i \\ &= TS - pV + \sum_i \mu_i n_i \end{aligned} \tag{3.69}$$

Taking the total differential of the above equation yields

$$dE = TdS + SdT - pdV - Vdp + \sum_i \mu_i dn_i + n_i d\mu_i$$

Comparison of Eqs. 3.68 and 3.70 gives the well-known *Gibbs-Duhem equation*

$$SdT - Vdp + \sum_i n_i d\mu_i = 0 \tag{3.70}$$

Another example is the classical and quantum mechanical *virial theorem* that uses homogeneity to relate the kinetic and potential energy. The virial theorem (for 1 particle) can be stated as

$$\left\langle x\frac{\partial V}{\partial x} + y\frac{\partial V}{\partial y} + z\frac{\partial V}{\partial z}\right\rangle = 2\langle K\rangle \tag{3.71}$$

Note that the factor 2 arises from the fact that the kinetic energy is a homogeneous functional of degree 2 in the particle coordinates. If the potential energy is a central potential; i.e., $V(r) = C \cdot r^n$ (a homogeneous functional of degree n) we obtain

$$n\langle V\rangle = 2\langle K\rangle \tag{3.72}$$

In the case of atoms (or molecules - if the above is generalized slightly) $V(r)$ is the Coulomb potential $1/r$, $n = -1$ and we have $< V >= -2 < K >$ or $E = (1/2) < V >$ since $E =< V > + < K >$.

3.5.2 Convexity properties of functions and functionals

Powerful relations can be derived for functions and functionals that possess certain *convexity* properties. We define convexity in three cases, starting with the most general: 1) general functions (functionals), 2) at least once-differentiable functions (functionals), and 3) at least twice-differentiable functions (functionals).

For a general function (functional) to be *convex* on the interval I (for functions) or the domain $\mathcal{D}$ (for functionals) if, for $0 \leq \lambda \leq 1$

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda)f(x_2) \tag{3.73}$$

$$F[\lambda f_1 + (1-\lambda)f_2] \leq \lambda F[f_1] + (1-\lambda)F[f_2] \tag{3.74}$$

for $x_1, x_2 \in I$ and $f_1, f_2 \in \mathcal{D}$. $f(x)$ ($F[f]$) is said to be *strictly convex* on the interval if the equality holds only for $x_1 = x_2$ ($f_1 = f_2$). $f(x)$ ($F[f]$) is said to be *concave* (*strictly concave*) if $-f(x)$ (-$F[f]$) is *convex* (*strictly convex*).

A once-differentiable function $f(x)$ (or functional $F[f]$) is convex if and only if

$$f(x_1) - f(x_2) - f'(x_2)\cdot(x_1 - x_2) \geq 0 \tag{3.75}$$

$$F[f_1] - F[f_2] - \int \left[\frac{\delta F[f]}{\delta f(x)}\right]_{f=f_2} (f_1(x) - f_2(x))\,dx \geq 0 \tag{3.76}$$

for $x_1, x_2 \in I$ and $f_1, f_2 \in \mathcal{D}$.

A twice-differentiable function $f(x)$ (or functional $F[f]$) is convex if and only if

$$f''(x) \geq 0 \quad (3.77)$$

$$\left[\frac{\delta^2 F[f]}{\delta f(x)\delta f(x')}\right] \geq 0 \quad (3.78)$$

for $x \in I$ and $f \in \mathcal{D}$.

An important property of convex functions (functionals) is known as *Jensen's inequality*: For a convext function $f(x)$ (functional $F[f]$)

$$f(\langle x\rangle) \leq \langle f(x)\rangle \quad (3.79)$$

$$F[\langle f\rangle] \leq \langle F[f]\rangle \quad (3.80)$$

where $\langle\cdots\rangle$ denotes an average (either discreet of continuous) over a positive semi-definite set of weights. In fact, Jensen's inequality can be extended to a convex function of a Hermitian operator

$$f\left(\left\langle\hat{O}\right\rangle\right) \leq \left\langle f(\hat{O})\right\rangle \quad (3.81)$$

where in this case $\langle\cdots\rangle$ denotes the quantum mechanical expectation value $\langle\Psi\mid\cdots\mid\Psi\rangle$. Hence, Jensen's inequality is valid for averages of the form

$$\langle f\rangle = \sum_i P_i f_i \text{ where } P_i \geq 0, \sum_i P_i = 1 \quad (3.82)$$

$$\langle f\rangle = \int P(x)f(x)\,dx; \text{ where } P(x) \geq 0, \int P(x)\,dx = 1 \quad (3.83)$$

$$\langle f\rangle = \int \Psi^*(x)\hat{f}\Psi(x)\,dx; \text{ where } \int \Psi^*(x)\Psi(x)\,dx = 1 \quad (3.84)$$

The proof is elementary but I don't feel like typing it at 3:00 in the morning. Instead, here is an example of an application - maybe in a later version...

Example: Convex functionals in statistical mechanics.

Consider the convect function e^x (it is an infinitely differentiable function, and has $d^2(e^x)/dx^2 = e^x$, a positive definite second derivative). Hence $e^{<x>} \leq \langle exp(x)\rangle$.

$$e^{<x>} \leq \langle exp(x)\rangle \quad (3.85)$$

This is a useful relation in statistical mechanics.

Similarly the function $xln(x)$ is convex for $x \geq 0$. If we consider two sets of probabilities P_i and P_i' such that $P_i, P_i' \geq 0$ and $\sum_i P_i = \sum_i P_i' = 1$, then we obtain from Jensen's inequality

$$\langle x\rangle\, ln(\langle x\rangle) \leq \langle xln(x)\rangle \quad (3.86)$$

$$\left(\sum_i^N P_i'\cdot\frac{P_i}{P_i'}\right) ln\left(\sum_i^N P_i'\cdot\frac{P_i}{P_i'}\right) \leq \left(\sum_i^N P_i'\cdot\frac{P_i}{P_i'}\cdot ln\left(\frac{P_i}{P_i'}\right)\right) \quad (3.87)$$

Note that $\sum_i^N P_i'\cdot P_i/P_i' = \sum_i^N P_i = 1$ and hence the left hand side of the above inequality is zero since $1\cdot ln(1) = 0$. The right hand side can be reduced by canceling out the P_i' factors in the numerator and denominator, which results in

$$\sum_i^N P_i\cdot ln\left(\frac{P_i}{P_i'}\right) \geq 0 \quad (3.88)$$

which is a famous inequality derived by Gibbs, and is useful in providing a lower bound on the entropy: let $P_i' = 1/N$ then, taking minus the above equation, we get

$$-\sum_i^N P_i\cdot ln\left(P_i\right) \leq ln(N) \quad (3.89)$$

If the entropy is defined as $-k_B\sum_i^N P_i\cdot ln\left(P_i\right)$ where k_B is the Boltzmann constant (a positive quantity), then the largest value the entropy can have (for an ensemble of N discreet states) is $k_B\cdot ln(N)$, which occurs when all probabilities are equal (the infinite temperature limit).

3.6 Lagrange Multipliers

In this section, we outline an elegant method to introduce constraints into the variational procedure. We begin with the case of a discreet constraint condition, and then outline the generalization to a continuous (pointwise) set of constraints.

Consider the problem to extremize the functional $F[f]$ subject to a functional constraint condition

$$G[f] = 0 \tag{3.90}$$

In this case, the *method of Lagrange multipliers* can be used. We define the auxiliary function

$$\Omega[f] \equiv F[f] - \lambda G[f] \tag{3.91}$$

where λ is a parameter that is yet to be determined. We then solve the variational condition

$$\frac{\delta \Omega}{\delta f(x)} = \frac{\delta F}{\delta f(x)} - \lambda \frac{\delta G}{\delta f(x)} = 0 \tag{3.92}$$

Solution of the above equation results, in general, in a infinite set of solutions depending on the continuous parameter $lambda$. We then have the freedom to choose the particular value of λ that satisfies the constraint requirement. Hopefully there exists such a value of λ, and that value is unique - but sometimes this is not the case. Note that, if $f_0(x)$ is a solution of the constrained variational equation (Eq. 3.92), then

$$\lambda = \left[\frac{\delta F}{\delta f(x)}\right]_{f=f_0} / \left[\frac{\delta G}{\delta f(x)}\right]_{f=f_0} \tag{3.93}$$

for *any and all* values of $f_0(x)$! Often in chemistry and physics the Lagrange multiplier itself has a physical meaning (interpretation), and is sometimes referred to as a *sensitivity coefficient*.

Constraints can be discreet, such as the above example, or continuous. A continuous (or *pointwise*) set of constraints can be written

$$g[f, x] = 0 \tag{3.94}$$

where the notation $g[f, x]$ is used to represent a simultaneous functional of f and function of x - alternately stated, $g[f, x]$ is a functional of f at every point x. We desire to impose a continuous set of constraints at every point x, and for this purpose, we require a Lagrange multiplier $\lambda(x)$ that is itself a continuous function of x. We then define (similar to the discreet constraint case above) the auxiliary function

$$\Omega[f] \equiv F[f] - \int \lambda(x) g[f, x]\, dx \tag{3.95}$$

and then solve

$$\frac{\delta \Omega}{\delta f(x)} = \frac{\delta F}{\delta f(x)} - \int \lambda(x') \frac{\delta g[f, x']}{\delta f(x)}\, dx' = 0 \tag{3.96}$$

As before, the Lagrange multiplier $\lambda(x)$ is determined to satisy the constraint condition of Eq. 3.94. One can consider $\lambda(x)$ to be a continuous (infinite) set of Lagrange multipliers associated with a constraint condition at each point x.

3.7 Problems

3.7.1 Problem 1

Consider the functional

$$T_W[\rho] = \frac{1}{8}\int \frac{\nabla\rho(\mathbf{r})\cdot\nabla\rho(\mathbf{r})}{\rho(\mathbf{r})} dddr \tag{3.97}$$

a. Evaluate the functional derivative $\delta T_W/\delta\rho(\mathbf{r})$.

b. Let $\rho(\mathbf{r}) = |\psi(\mathbf{r})|^2$ (assume ψ is real), and rewrite $T[\psi] = T_W[|\psi(\mathbf{r})|^2]$. What does this functional represent in quantum mechanics?

c. Evaluate the functional derivative $\delta T[\psi]/\delta\psi(\mathbf{r})$ directly and verify that it is identical to the functional derivative obtained using the chain relation

$$\frac{\delta T[\psi]}{\delta\psi(\mathbf{r})} = \frac{\delta T_W[\rho]}{\delta\psi(\mathbf{r})} = \int \frac{\delta T_W[\rho]}{\delta\rho(\mathbf{r}')}\cdot\frac{\delta\rho(\mathbf{r}')}{\delta\psi(\mathbf{r})} d^3r'$$

3.7.2 Problem 2

Consider the functional

$$E_x[\rho] = -\int \rho^{4/3}(\mathbf{r})\left[c - b^2 x^{3/2}(\mathbf{r})\right] d^3r \tag{3.98}$$

where c and b are constants, and

$$x(\mathbf{r}) = \frac{|\nabla\rho(\mathbf{r})|}{\rho^{4/3}(\mathbf{r})} \tag{3.99}$$

evaluate the functional derivative $\frac{\delta E_x[\rho]}{\delta\rho(\mathbf{r})}$.

3.7.3 Problem 3

This problem is an illustrative example of variational calculus, vector calculus and linear algebra surrounding an important area of physics: classical electrostatics.

The classical electrostatic energy of a charge distribution $\rho(\mathbf{r})$ is given by

$$J[\rho] = \frac{1}{2}\int\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r d^3r' \tag{3.100}$$

This is an example of a homogeneous functional of degree 2, that is to say $J[\lambda\rho] = \lambda^2 J[\rho]$.

3.7.3.1 Part A

Show that

$$J[\rho] = \frac{1}{k}\int \left[\frac{\delta J}{\delta\rho(\mathbf{r})}\right]_\rho \rho(\mathbf{r}) d^3r \tag{3.101}$$

where $k = 2$. Show that the quantity $\left[\frac{\delta J}{\delta\rho(\mathbf{r})}\right]_\rho = \phi(\mathbf{r})$ where $\phi(\mathbf{r})$ is the electrostatic potential due to the charge distribution $\rho(\mathbf{r})$.

3.7.3.2 Part B

The charge density $\rho(\mathbf{r})$ and the the electrostatic potential $\phi(\mathbf{r})$ are related by formula derived above. With appropriate boundary conditions, an equivalent condition relating $\rho(\mathbf{r})$ and $\phi(\mathbf{r})$ is given by the Poisson equation

$$\nabla^2\phi(\mathbf{r}) = -4\pi\rho(\mathbf{r})$$

Using the Poisson equation and Eq. 3.101 above, write a new functional $W_1[\phi]$ for the electrostatic energy with ϕ as the argument instead of ρ and calculate the functional derivative $\frac{\delta W_1}{\delta\phi(\mathbf{r})}$.

3.7.3.3 Part C

Rewrite $W_1[\phi]$ above in terms of the electrostatic (time independant) field $\mathbf{E} = -\nabla\phi$ assuming that the quantity $\phi(\mathbf{r})\nabla\phi(\mathbf{r})$ vanishes at the boundary (e.g., at $|\mathbf{r}| = \infty$). Denote this new functional $W_2[\phi]$. $W_2[\phi]$ should have no explicit dependence on ϕ itself, only through terms involving $\nabla\phi$.

3.7.3.4 Part D

Use the results of the Part C to show that

$$J[\rho] = W_1[\phi] = W_2[\phi] \geq 0$$

for any ρ and ϕ connected by the Poisson equation and subject to the boundary conditions described in Part C. **Note:** $\rho(\mathbf{r})$ can be either positive OR negative or zero at different $\mathbf{r}$.

3.7.3.5 Part E

Show explicitly

$$\frac{\delta W_1}{\delta\phi(\mathbf{r})} = \frac{\delta W_2}{\delta\phi(\mathbf{r})}$$

3.7.4 Problem 4

This problem is a continuation of problem 3.

3.7.4.1 Part F

Perform an integral Taylor expansion of $J[\rho]$ about the reference charge density $\rho_0(\mathbf{r})$. Let $\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0(\mathbf{r})$. Similarly, let $\phi(\mathbf{r})$, $\phi_0(\mathbf{r})$ and $\delta\phi(\mathbf{r})$ be the electrostatic potentials associated with $\rho(\mathbf{r})$, $\rho_0(\mathbf{r})$ and $\delta\rho(\mathbf{r})$, respectively.

Write out the Taylor expansion to infinite order. This is not an infinite problem! At what order does the Taylor expansion become *exact* for *any* $\rho_0(\mathbf{r})$ that is sufficiently smooth?

3.7.4.2 Part G

Suppose you have a density $\rho(\mathbf{r})$, but you *do not know* the associated electrostatic potential $\phi(\mathbf{r})$. In other words, for some reason it is not convenient to calculate $\phi(\mathbf{r})$ via

$$\phi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r$$

However, suppose you know a density $\rho_0(\mathbf{r})$ that closely resembles $\rho(\mathbf{r})$, and for which you *do know* the associated electrostatic potential $\phi_0(\mathbf{r})$. So the knowns are $\rho(\mathbf{r})$, $\rho_0(\mathbf{r})$ and $\phi_0(\mathbf{r})$ (but NOT $\phi(\mathbf{r})$!) and the goal is to approximate $J[\rho]$ in the best way possible from the knowns. Use the results of Part F to come up with a new functional $W_3[\rho, \rho_0, \phi_0]$ for the *approximate* electrostatic energy in terms of the known quantities.

3.7.4.3 Part H

Consider the functional

$$U_\phi[\tilde{\phi}] = \int \rho(\mathbf{r})\tilde{\phi}(\mathbf{r})d^3r + \frac{1}{8\pi}\int \tilde{\phi}(\mathbf{r})\nabla^2\tilde{\phi}(\mathbf{r})d^3r \tag{3.102}$$

where $\tilde{\phi}(\mathbf{r})$ is *not* necessarily the electrostatic potential corresponding to $\rho(\mathbf{r})$, but rather a trial function independent of $\rho(\mathbf{r})$. Show that

$$\frac{\delta U_\phi[\tilde{\phi}]}{\delta\tilde{\phi}(\mathbf{r})} = 0$$

leads to the Poisson equation; i.e., the $\tilde{\phi}(\mathbf{r})$ that produces an extremum of $U_\phi[\tilde{\phi}]$ is, in fact, the electrostatic potential $\phi(\mathbf{r})$ corresponding to $\rho(\mathbf{r})$.

Note: we could also have written the functional $U_\phi[\tilde{\phi}]$ in terms of the trial density $\tilde{\rho}(\mathbf{r})$ as

$$U_\rho[\tilde{\rho}] = \int\int \frac{\rho(\mathbf{r})\tilde{\rho}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3rd^3r' - \frac{1}{2}\int\int \frac{\tilde{\rho}(\mathbf{r})\tilde{\rho}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3rd^3r' \tag{3.103}$$

withe the variational condition

$$\frac{\delta U_\rho[\tilde{\rho}]}{\delta\tilde{\rho}(\mathbf{r})} = 0$$

3.7.4.4 Part I

Show that $U_\phi[\phi_0]$ and $U_\rho[\rho_0]$ of Part H are equivalent to the expression for $W_3[\rho,\rho_0,\phi_0]$ in Part G. In other words, the functional $W_3[\rho,\rho_0,\phi_0]$ shows you how to obtain the "best" electrostatic energy approximation for $J[\rho]$ given a reference density $\rho_0(\mathbf{r})$ for which the electrostatic potential $\phi_0(\mathbf{r})$ is known. The variational condition $\frac{\delta U_\phi[\tilde{\phi}]}{\delta\tilde{\phi}(\mathbf{r})} = 0$ or $\frac{\delta U_\rho[\tilde{\rho}]}{\delta\tilde{\rho}(\mathbf{r})} = 0$ of Part H provides a prescription for obtaining the "best" possible model density and model potential $\tilde{\phi}(\mathbf{r})$. *This is really useful!!*

3.7.4.5 Part J

We now turn toward casting the variational principle in Part H into linear-algebraic form. We first expand the trial density $\tilde{\rho}(\mathbf{r})$ as

$$\tilde{\rho}(\mathbf{r}) = \sum_k^{N_f} c_k\rho_k(\mathbf{r})$$

where the $\rho_k(\mathbf{r})$ are just a set of N_f analytic functions (say Gaussians, for example) for which it assumed we can solve or in some other way conveniently obtain the matrix elements

$$A_{i,j} = \int\int \frac{\rho_i(\mathbf{r})\rho_j(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3rd^3r'$$

and

$$b_i = \int\int \frac{\rho(\mathbf{r})\rho_i(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3rd^3r'$$

so $\mathbf{A}$ is an $N_f \times N_f$ square, symmetric matrix and $\mathbf{b}$ is an $N_f \times 1$ column vector. Rewrite $U_\rho[\tilde{\rho}]$ of Part I as a matrix equation $U_\rho[\mathbf{c}]$ involving the $\mathbf{A}$ matrix and $\mathbf{b}$ vector defined above. Solve the equation

$$\frac{\delta U_\rho[\mathbf{c}]}{\delta\mathbf{c}} = 0$$

for the coefficient vector $\mathbf{c}$ to give the "best" model density $\tilde{\rho}(\mathbf{r})$ (in terms of the electrostatic energy).

3.7.4.6 Part K

Repeat the excercise in Part J with an additional constraint that the model density $\tilde{\rho}(\mathbf{r})$ have the same normalization as the real density $\rho(\mathbf{r})$; i.e., that

$$\int \tilde{\rho}(\mathbf{r})d^3r = \int \rho(\mathbf{r})d^3r = N \tag{3.104}$$

or in vector form

$$\mathbf{c}^T \cdot \mathbf{d} = N \tag{3.105}$$

where $d_i = \int \rho_i(\mathbf{r})d^3r$. In other words, solve

$$\delta \left\{ U_\rho[\mathbf{c}] - \lambda(\mathbf{c}^T \cdot \mathbf{d} - N) \right\} = 0$$

for $\mathbf{c}^*(\lambda)$ in terms of the parameter λ, and determine what value of the Lagrange multiplier λ satisfies the constraint condition of Eq. 3.105.

3.7.4.7 Part L

In Part J you were asked to solve an *unconstrained* variational equation, and in Part K you were asked to solve for the more general case of a variation with a single constraint. 1) Show that the general solution of $\mathbf{c}^*(\lambda)$ (the $*$ superscript indicates that $\mathbf{c}^*(\lambda)$ variational solution and not just an arbitrary vector) of Part K reduces to the unconstrained solution of Part J for a particular value of λ (which value?). 2) Express $\mathbf{c}^*(\lambda)$ as $\mathbf{c}^*(\lambda) = \mathbf{c}^*(0) + \delta\mathbf{c}^*(\lambda)$ where $\delta\mathbf{c}^*(\lambda)$ is the unconstrained variational solution $\mathbf{c}^*(0)$ when the constraint condition is turned on. Show that indeed, $U_\rho[\mathbf{c}^*(0)] \geq U_\rho[\mathbf{c}^*(\lambda)]$. Note that this implies the extremum condition corresponds to a *maximum*. 3) Suppose that the density $\rho(\mathbf{r})$ you wish to model by $\tilde{\rho}(\mathbf{r})$ can be represented by

$$\rho(\mathbf{r}) = \sum_k x_k \rho_k(\mathbf{r}) \tag{3.106}$$

where the functions $\rho_k(\mathbf{r})$ are the same functions that were used to expand $\tilde{\rho}(\mathbf{r})$. Explicitly solve for $\mathbf{c}^*(0)$, λ and $\mathbf{c}^*(\lambda)$ for this particular $\rho(\mathbf{r})$.

3.7.4.8 Part M

In Part J you were asked to solve an *unconstrained* variational equation, and in Part K you were asked to solve for the more general case of a variation with a single constraint. You guessed it - now we generalize the solution to an *arbitrary number of constraints* (so long as the number of constraints N_c does not exceed the number of variational degrees of freedom N_f - which we henceforth will assume). For example, we initially considered a single normalization constraint that the model density $\tilde{\rho}(\mathbf{r})$ integrate to the same number as the reference density $\rho(\mathbf{r})$, in other words

$$\int \tilde{\rho}(\mathbf{r})d^3r = \int \rho(\mathbf{r})d^3r \equiv N$$

This constraint is a specific case of more general form of *linear* constraint

$$\int \tilde{\rho}(\mathbf{r})f_n(\mathbf{r})d^3r = \int \rho(\mathbf{r})f_n(\mathbf{r})d^3r \equiv y_n$$

For example, if $f_1(\mathbf{r}) = 1$ we recover the original constraint condition with $y_1 = N$, which was that the *monopole* moment of $\tilde{\rho}$ equal that of ρ. As further example, if $f_2(\mathbf{r}) = x$, $f_3(\mathbf{r}) = y$, and $f_4(\mathbf{r}) = z$, then we would also require that each component of the *dipole* moment of $\tilde{\rho}$ equal those of ρ, and in general, if $f_n(\mathbf{r}) = r^l Y_{lm}(\hat{\mathbf{r}})$

where the functions Y_{lm} are spherical harmonics, we could constrain an arbitrary number of *multipole moments* to be identical.

This set of N_c constraint conditions can be written in matrix form as

$$\mathbf{D}^T \cdot \mathbf{c} = \mathbf{y}$$

where the matrix $\mathbf{D}$ is an $N_f \times N_c$ matrix defined as

$$D_{i,j} = \int \rho_i(\mathbf{r}) f_j(\mathbf{r}) d^3r$$

and the $\mathbf{y}$ is an $N_c \times 1$ column vector defined by

$$y_j = \int \rho(\mathbf{r}) f_j(\mathbf{r}) d^3r$$

Solve the general constrained variation

$$\delta \left\{ U_\rho[\mathbf{c}] - \boldsymbol{\lambda}^T \cdot (\mathbf{D}^T \cdot \mathbf{c} - \mathbf{y}) \right\} = 0$$

for the coefficients $\mathbf{c}^*(\boldsymbol{\lambda})$ and the $N_c \times 1$ *vector* of Lagrange multipliers $\boldsymbol{\lambda}$. Verify that 1) if $\boldsymbol{\lambda} = 0$ one recovers the unconstrained solution of Part J, and 2) $\boldsymbol{\lambda} = \lambda \mathbf{1}$ (where $\mathbf{1}$ is just a vector of 1's) recovers the solution for the single constraint condition of Part K.

Chapter 4

Elementary Principles of Classical Mechanics

4.1 Mechanics of a system of particles

4.1.1 Newton's laws

1. Every object in a state of uniform motion tends to remain in that state unless acted on by an external force.

$$\mathbf{v}_i = \dot{\mathbf{r}}_i = \frac{d}{dt}\mathbf{r}_i \tag{4.1}$$

$$\mathbf{p}_i = m_i\dot{\mathbf{r}}_i = m_i\mathbf{v}_i \tag{4.2}$$

2. The force is equal to the change in momentum per change in time.

$$\mathbf{F}_i = \frac{d}{dt}\mathbf{p}_i \equiv \dot{\mathbf{p}}_i \tag{4.3}$$

3. For every action there is an equal and opposite reaction.

$$\mathbf{F}_{ij} = -\mathbf{F}_{ij} \text{ (weak law), not always true}$$

e.g. $\mathbf{F}_{ij} = -\nabla_i V(\mathbf{r}_{ij})$, e.g. Biot-Savart law moving e^-

$$\mathbf{F}_{ij} = f_{ij}\mathbf{r}_{ij} = -\mathbf{F}_{ij} = f_{ji}\mathbf{r}_{ji} \text{ (strong law)}$$

e.g. $\mathbf{F}_{ij} = -\nabla_i V(|\mathbf{r}_{ij}|)$, e.g. "Central force problem"

4.1.2 Fundamental definitions

$$\mathbf{v}_i = \frac{d}{dt}\mathbf{r}_i \equiv \dot{\mathbf{r}}_i \tag{4.4}$$

$$\mathbf{a}_i = \frac{d}{dt}\mathbf{v}_i = \frac{d^2}{dt^2}\mathbf{r}_i = \dot{\mathbf{r}}_i \tag{4.5}$$

$$\mathbf{p}_i = m_i\mathbf{v}_i = m_i\dot{\mathbf{r}}_i \tag{4.6}$$

$$\mathbf{L}_i = \mathbf{r}_i \times \mathbf{p}_i \tag{4.7}$$

$$\mathbf{N}_i = \mathbf{r}_i \times \mathbf{F}_i = \dot{\mathbf{L}}_i \tag{4.8}$$

$$\mathbf{F}_i = \dot{\mathbf{p}}_i = \frac{d}{dt}(m_i\dot{\mathbf{r}}_i) \tag{4.9}$$

$$\begin{aligned}\mathbf{N}_i &= \mathbf{r}_i \times \mathbf{p}_i \\ &= \mathbf{r}_i \times \frac{d}{dt}(m_i\dot{\mathbf{r}}_i) \\ &= \frac{d}{dt}(\mathbf{r}_i \times \mathbf{p}_i) \\ &= \frac{d}{dt}\mathbf{L}_i \\ &= \dot{\mathbf{L}}_i\end{aligned} \tag{4.10}$$

Proof:

$$\begin{aligned}\frac{d}{dt}(\mathbf{r}_i \times \mathbf{p}_i) &= \dot{\mathbf{r}}_i \times \mathbf{p}_i + \mathbf{r}_i \times \dot{\mathbf{p}}_i \\ &= \mathbf{v}_i \times m\mathbf{v}_i + \mathbf{r}_i \times \dot{\mathbf{p}}_i \\ &= 0 + \mathbf{r}_i \times \dot{\mathbf{p}}_i\end{aligned} \tag{4.11}$$

If $\frac{d}{dt}A(t) = 0$, $At =$constant, and A is “conserved.”

A “conservative” force field (or system) is one for which the work required to move a particle in a closed loop vanishes.

$\oint \mathbf{F} \cdot d\mathbf{s} = 0$ note: $\mathbf{F} = \nabla V(\mathbf{r})$, then

$$\oint_c -\nabla V(\mathbf{r}) \cdot d\mathbf{s} = \int_s -(\underbrace{\boldsymbol{\nabla} \times \boldsymbol{\nabla} V(\mathbf{r})}_{\theta}) \cdot \hat{n} da \tag{4.12}$$

$$\oint_c \mathbf{A} \cdot d\mathbf{s} = \int_s (\boldsymbol{\nabla} \times \mathbf{A}) \cdot \hat{n} da \quad \text{(Stoke's Theorem)} \tag{4.13}$$

System of particles $m_i \neq m_i(t)$

Fixed mass, strong law of a and r on internal forces.

Suppose $\mathbf{F}_i = \sum_j \mathbf{F}_{ji} + \mathbf{F}_i^{(e)}$ and $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$

$$\mathbf{F}_{ij} = 0$$

$$\mathbf{r}_{ij} \times \mathbf{F}_{ij} = \mathbf{r}_{ji} \times \mathbf{F}_{ji} = 0 \tag{4.14}$$

Strong law on $\mathbf{F}_{ij}$

$$\begin{aligned}\mathbf{F}_i = \mathbf{P}_i =& \frac{d}{dt}\left(m_i \frac{d}{dt}\mathbf{r}_i\right) \\ =& \frac{d^2}{dt^2} m_i \mathbf{r}_i, \text{ for } m_i \neq m_i(t)\end{aligned} \tag{4.15}$$

let $\mathbf{R} = \frac{\sum_i m_i \mathbf{r}_i}{M}$ and $M = \sum_i m_i$

$$\begin{aligned}\sum_i \mathbf{F}_i =& \frac{d^2}{dt^2}\sum_i m_i \mathbf{r}_i \\ =& M\frac{d^2}{dt^2}\sum_i \frac{m_i \mathbf{r}_i}{M} \\ =& M\frac{d^2\mathbf{R}}{dt^2} \\ =& \sum_i \mathbf{F}_i^{(e)} + \sum_i \sum_j \mathbf{F}_{ij}\end{aligned} \tag{4.16}$$

Note: $\sum_i \sum_j \mathbf{F}_{ij} = \sum_i \sum_{j>i} (\mathbf{F}_{ij} + \mathbf{F}_{ji}) = 0$

$$\dot{\mathbf{P}} \equiv M\frac{d^2\mathbf{R}}{dt^2} = \sum_i \mathbf{F}_i^{(e)} \equiv \mathbf{F}^{(e)} \tag{4.17}$$

$$\begin{aligned}\dot{\mathbf{P}} =& \sum_i M\frac{d\mathbf{r}_i}{dt} \\ =& \frac{d}{dt}\mathbf{P}\end{aligned} \tag{4.18}$$

$$\begin{aligned}\mathbf{N}_i =& \mathbf{r}_i \times \mathbf{F}_i \\ =& \mathbf{r}_i \times \dot{\mathbf{P}}_i \\ =& \dot{\mathbf{L}}_i\end{aligned} \tag{4.19}$$

$$\begin{aligned}\mathbf{N}_i =& \sum_i \mathbf{N}_i = \sum_i \dot{\mathbf{L}}_i = \dot{\mathbf{L}} \\ =& \sum_i \mathbf{r}_i \times \mathbf{F}_i = \sum_i \mathbf{r}_i \times \left(\sum_j \mathbf{F}_{ji} + \mathbf{F}_i^{(e)}\right) \\ =& \sum_{ij} \mathbf{r}_i \times \mathbf{F}_{ji} + \sum_i \mathbf{r}_i \times \mathbf{F}_i^{(e)} \\ =& \sum_i \mathbf{r}_i \times \mathbf{F}_i^{(e)} = \mathbf{N}^{(e)} = \dot{\mathbf{L}}_i\end{aligned} \tag{4.20}$$

$$\sum_i \sum_{j<i} \mathbf{r}_i \times \mathbf{F}_{ij} + \sum_i \sum_{j>i} \mathbf{r}_i \times \mathbf{F}_{ji} = 0 \tag{4.21}$$
$$\sum_i \sum_{j<i} \mathbf{r}_i \times \mathbf{F}_{ij} = -\sum_i \sum_{j>i} \mathbf{r}_i \times \mathbf{F}_{ji}$$

Note, although

$$\begin{aligned} \mathbf{P} &= \sum_i P_i \\ &= \sum_i m_i \frac{d}{dt}\mathbf{r}_i \\ &= m\frac{d}{dt} \end{aligned} \tag{4.22}$$

$$\tag{4.23}$$

$$\mathbf{V} \equiv \frac{d\mathbf{R}}{dt} \neq \sum_i \mathbf{v}_i = \sum_i \frac{d\mathbf{r}_i}{dt}$$

$$\begin{aligned} \mathbf{L} &= \sum_i \mathbf{L}_i \\ &= \sum_i \mathbf{r}_i \times \mathbf{P}_i \end{aligned} \tag{4.24}$$

$$\mathbf{r}_i = (\mathbf{r}_i - \mathbf{R}) + \mathbf{R} = \mathbf{r}'_i + \mathbf{R} \tag{4.25}$$
$$\dot{\mathbf{r}}_i = \dot{\mathbf{r}}'_i + \dot{\mathbf{R}} \tag{4.26}$$

$$\mathbf{p}_i = \mathbf{p}'_i + m_i\mathbf{V} \tag{4.27}$$
$$(\mathbf{V}_i = \mathbf{V}'_i + \mathbf{V}) \tag{4.28}$$

$$\mathbf{L} = \sum_i \mathbf{r}'_i \times \mathbf{P}'_i + \sum_i \mathbf{R}_i \times \mathbf{P}'_i + \sum_i \mathbf{r}'_i \times m_i\mathbf{V}_i + \sum_i \mathbf{R}_i \times m_i\mathbf{V}_i \tag{4.29}$$

Note

$$\begin{aligned} \sum_i m_i\mathbf{r}'_i &= \sum_i m_i\mathbf{r}_i - \sum_i m_i\mathbf{R} \\ &= M\mathbf{R} - M\mathbf{R} = 0 \end{aligned} \tag{4.30}$$

hence

$$\sum_i \mathbf{r}_i \times m_i\mathbf{V} = \left(\sum_i m_i\mathbf{r}_i\right) \times \mathbf{V} = 0 \tag{4.31}$$

$$\begin{aligned} \sum_i \mathbf{R} \times \mathbf{P}'_i &= \sum_i \mathbf{R} \times m_i\mathbf{V}'_i \\ &= \mathbf{R} \times \frac{d}{dt}\left(\sum_i m_i\mathbf{r}'_i\right) \\ &= 0 \end{aligned} \tag{4.32}$$

$$\mathbf{L} = \underbrace{\sum_i \mathbf{r}'_i \times \mathbf{P}'_i}_{\mathbf{L}\text{ about C.O.M.}} + \underbrace{\mathbf{R} \times M\mathbf{V}}_{\mathbf{L}\text{ of C.O.M.}} \tag{4.33}$$

For a system of particles obeying Newton's equations of motion, the work done by the system equals the difference in kinetic energy.

$$\mathbf{F}_i = m_i \dot{\mathbf{V}}_i, d\mathbf{r}_i = \frac{d\mathbf{r}_i}{dt} dt \tag{4.34}$$

$$\begin{aligned} W_{12} &= \sum_i \int_1^2 F_i \cdot d\mathbf{r}_i \\ &= \sum_i \int_1^2 m_i \dot{\mathbf{V}}_i \cdot \mathbf{V}_i dt \\ &= \sum_i \int_1^2 \frac{1}{2} m_i \frac{d}{dt} (\mathbf{V}_i \cdot \mathbf{V}_i) dt \\ &= \sum_i \frac{1}{2} m_i \mathbf{V}_i \cdot \mathbf{V}_i \Big|_1^2 = \frac{1}{2} m_i \mathbf{V}_i^2 \Big|_1^2 = T_2 - T_1 \end{aligned} \tag{4.35}$$

The kinetic energy can be expressed as a kinetic energy of the center of mass and a T of the particles relative to the center of mass.

$$\begin{aligned} T &= \frac{1}{2} \sum_i m_i (\mathbf{V} + \mathbf{V}'_i) \cdot (\mathbf{V} + \mathbf{V}'_i) \\ &= \underbrace{\frac{1}{2} \sum_i m_i V^2}_{\frac{1}{2} M V^2} + \underbrace{\sum_i m_i \mathbf{V}'_i \cdot \mathbf{V}}_{(\sum_i m_i \mathbf{V}'_i) \cdot \mathbf{V}} + \underbrace{\frac{1}{2} \sum_i m_i (\mathbf{V}'_i)^2}_{\text{internal}} \end{aligned} \tag{4.36}$$

Note

$$\sum_i m_i \mathbf{V}'_i = \sum_i m_i \mathbf{V}_i - M\mathbf{V} = 0$$

Proof

$$\begin{aligned} \sum_i m_i \mathbf{V}'_i &= \frac{d}{dt} \sum_i m_i \mathbf{r}_i \\ &= M \frac{d}{dt} \sum_i \frac{m_i \mathbf{r}_i}{M} \\ &= M \frac{d\mathbf{R}}{dt} \\ &= M\mathbf{V} \end{aligned} \tag{4.37}$$

$$W_{12} = T_2 - T_1 = \sum_i \int_1^2 \mathbf{F}_i \cdot d\mathbf{r}_i \tag{4.38}$$

In the special case that

$$\mathbf{F}_i = \mathbf{F}_i^{(e)} + \sum_j \mathbf{F}_{ij} \text{ where } \mathbf{F}_i^{(e)} = -\nabla_i V_i \text{ and } \mathbf{F}_{ij} = -\nabla_i V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|)$$

Note

$$\begin{aligned} -\nabla_i V_{ij}(r_{ij}) =& \nabla_j V_i, V_{ij}(r_{ij}) \\ =& V_{ji}(r_{ij}) \\ =& \frac{-1}{r_{ij}}\left(\frac{dV}{dr_{ij}}\right)(\mathbf{r}_i - \mathbf{r}_j) \\ =& -\mathbf{F}_{ji} \end{aligned} \tag{4.39}$$

$$\begin{aligned} W_{12} =& T_2 - T_1 \\ =& \sum_i \int_1^2 -\nabla_i V_i \cdot d\mathbf{r}_i + \sum_i \sum_j \int_1^2 -\nabla_i V_{ij}(r_{ij}) \cdot f\mathbf{r}_i \end{aligned} \tag{4.40}$$

Note

$$\begin{aligned} \int_1^2 \nabla_i V_i \cdot d\mathbf{r}_i =& -\int_1^2 (d\mathbf{r}_i \cdot \nabla_i) V_i \\ =& -\int_1^2 dV_i = V_i\Big|_1^2 \end{aligned} \tag{4.41}$$

where

$$d\mathbf{r}_i \cdot \nabla_i = dx\frac{d}{dx} + dy\frac{d}{dy} + dz\frac{d}{dz} \tag{4.42}$$

$$\sum_i \sum_j A_{ij} = \sum_i \sum_{j<i} A_{ij} + \sum_i \sum_{j>i} A_{ji} + \sum_i A_{ii} \tag{4.43}$$

$$\begin{aligned} -\sum_i \sum_j \int_1^2 \nabla_i V_{ij} r_{ij} \cdot d\mathbf{r}_i =& -\sum_i \sum_{j<i} \int_1^2 \nabla_i V_{ij}(r_{ij}) \cdot d\mathbf{r}_i \nabla_j V_{ji}(r_{ij}) \cdot d\mathbf{r}_j \\ =& -\sum_i \sum_{j<i} \int_1^2 \nabla_{ij} V_{ij}(r_{ij}) d\mathbf{r}_{ij} \\ =& -\sum_i \sum_{j<i} \int_1^2 (d\mathbf{r}_{ij} \cdot \nabla_{ij}) V_{ij} \\ =& -\sum_i \sum_{j<i} \int_1^2 dV_{ij} \\ =& -\sum_i \sum_{j<i} V_{ij}\Big|_1^2 \\ =& -\frac{1}{2} \sum_i \sum_j V_{ij}\Big|_1^2 \end{aligned} \tag{4.44}$$

Hence we can define a potential energy

$$V = \underbrace{\sum_i V_i}_{\text{external}} + \underbrace{\frac{1}{2}\sum_{ij} V_{ij}}_{\text{internal}} \tag{4.45}$$

$$\begin{aligned} W_{12} =& T_2 - T_1 \\ =& -(V_2 - V_1) \\ =& V_1 - V_2 \end{aligned} \tag{4.46}$$

4.2 Constraints

Constraints are scleronomous if they do not depend explicitly on time, and are rheonomous if they do.

$(f\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) = 0$ (holonomic)

e.g. rigid body $(\mathbf{r}_i - \mathbf{r}_j)^2 = C_{ij}^2$
Nonholonomic: $r^2 a^2 \geq 0$, e.g. container boundary

Nonholonomic constaints cannot be used to eliminate dependent variables.

$$\mathbf{r}_1 \ldots \mathbf{r}_N \rightarrow \mathbf{q}_1 \ldots \mathbf{q}_{N-K}; \mathbf{q}_{N-K+1} \cdots \mathbf{q}_N$$

For holonomic systems with applied forces derivable from a scalar potential with workless constraints, a Lagrangian can always be defined.

“Constraints” are artificial...name one that is not...?

$$\mathbf{r}_i(q_1, q_2 \ldots q_{N-K}, t; q_{N-K+1}, q_N)$$

4.3 D’Alembert’s principle

$$\mathbf{F}_i = \mathbf{F}_i^{(a)} + \mathbf{f}_i \qquad \begin{aligned} \mathbf{F}_i^{(a)} =& \text{ applied force} \\ \mathbf{f}_i =& \text{ constraint force} \end{aligned}$$

$\delta\mathbf{r}_i(t)$ = virtual (infintesimal) displacement, so small that $\mathbf{F}_i$ does not change, consistent with the forces and constraints at the time t.

We consider only constraint forces $\mathbf{f}_i$ that do no net virtual work on the system $(\sum_i \mathbf{f}_i \cdot \mathbf{v}_i = 0)$ since:

$$\begin{aligned} W_{12} =& \int_1^2 \mathbf{f}_i \cdot d\mathbf{r}_i \\ =& \int_1^2 \mathbf{f}_i \cdot \mathbf{v}_i dt \end{aligned} \tag{4.47}$$

In other words, infintesimally, $\sum_i \mathbf{f}_i \cdot \delta\mathbf{r}_i = 0$.

Not all constraint forces obey this condition, like a frictional force due to sliding on a surface.

So at equilibrium, $\mathbf{F}_i = 0$, thus

$$\begin{aligned} \sum_i \mathbf{F}_i \cdot \delta\mathbf{r}_i =& \sum_i \mathbf{F}_i^{(a)} \cdot \delta\mathbf{r}_i + \sum_i \mathbf{f}_i \cdot \delta\mathbf{r}_i \\ =& \sum_i \mathbf{F}_i^{(a)} \cdot \delta\mathbf{r}_i \end{aligned} \tag{4.48}$$

The principle of virtual work for a system at equilibrium:

$$\sum_i \mathbf{F}_i^{(a)} \cdot \delta \mathbf{r}_i = 0 \tag{4.49}$$

We want to derive Lagrange's equations for a set of generalized corrdinates that can be used to eliminate a set of holonomic constraints. Here we go. . . we start with Newton's equations (valid for Cartesian Coordinates)

$$\mathbf{F}_i = \dot{\mathbf{P}}_i, \text{ or } (\mathbf{F}_i - \dot{\mathbf{P}}_i) = 0$$

$$\sum_i (\mathbf{F}_i - \dot{\mathbf{P}}_i) \cdot \delta \mathbf{r}_i = 0 \tag{4.50}$$

Recall $\delta \mathbf{r}_i$ is not an independent variation-it must obey the constraints.

D'Alembert's principle:

$$\sum_i \left(\mathbf{F}_i^{(a)} - \dot{\mathbf{P}}_i \right) \cdot \delta \mathbf{r}_i + \sum_i \mathbf{f}_i \cdot \delta \mathbf{r}_i = \sum_i \left(\mathbf{F}_i^{(a)} - \dot{\mathbf{P}}_i \right) \cdot \delta \mathbf{r}_i = 0 \tag{4.51}$$

(for constant forces that do no net virtual work)

Not useful yet. . .

$$\mathbf{r}_i = \mathbf{r}_i(q_1, q_2, \ldots, q_N, t)$$

$$\begin{aligned} \mathbf{v}_i &= \frac{d}{dt}\mathbf{r}_i \\ &= \sum_j \frac{\partial \mathbf{r}_i}{\partial q_j} \frac{dq_j}{dt} + \frac{\partial \mathbf{r}_i}{\partial t} \\ &= \sum_j \frac{\partial \mathbf{r}_i}{\partial q_j} \dot{q}_j + \frac{\partial \mathbf{r}_i}{\partial t} \end{aligned} \tag{4.52}$$

$$\delta \mathbf{r}_i = \sum_j \frac{\partial \mathbf{r}_i}{\partial q_j} \delta q_j \tag{4.53}$$

$$\begin{aligned} \sum_i \mathbf{F}_i \cdot \delta \mathbf{r}_i &= \sum_i \sum_j \mathbf{F}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \\ &= \sum_j Q_j \delta q_j \end{aligned} \tag{4.54}$$

Where $Q_j \equiv \sum_i \mathbf{F}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j}$ = generalized force.

$$\begin{aligned} \sum_i \dot{\mathbf{P}}_i \cdot \delta \mathbf{r}_i &= \sum_i m_i \ddot{\mathbf{r}}_i \\ &= \sum_{i,j} m_i \ddot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \delta q_j \end{aligned} \tag{4.55}$$

Note:

$$\sum_i \frac{d}{dt}\left(m_i \dot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j}\right) = \sum_i m_i \ddot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} + m_i \dot{\mathbf{r}}_i \cdot \frac{d}{dt}\left(\frac{\partial \mathbf{r}_i}{\partial q_j}\right)$$

and, $\frac{d}{dt}\left(\frac{\partial \mathbf{r}_i}{\partial q_j}\right) = \frac{\partial \mathbf{v}_i}{\partial q_j}$; recall $\frac{\partial \mathbf{v}_i}{\partial \dot{q}_j} = \frac{\partial \mathbf{r}_i}{\partial q_j}$

$$\begin{aligned} \sum_i \dot{\mathbf{P}}_i \cdot \delta \mathbf{r}_i &= \sum_{i\,,\,j} \left[\underbrace{\frac{d}{dt}\left(m_i \mathbf{v}_i \cdot \frac{\partial \mathbf{v}_i}{\partial \dot{q}_j}\right)}_{\frac{\partial}{\partial \dot{q}_j}\left(\frac{1}{2} m_i v_i^2\right)} - \underbrace{m_i \mathbf{v}_i \cdot \frac{\partial \mathbf{v}_i}{\partial q_j}}_{\frac{\partial}{\partial q}\left(\frac{1}{2} m_i v_i^2\right)} \right] \delta q_j \\ &= \sum_j \left[\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q}\right] \cdot \delta q_j \end{aligned} \tag{4.56}$$

So D'Alembert's principle can be written:

$$-\sum_i \left(\mathbf{F}_i^{(a)} - \dot{\mathbf{P}}_i\right) \cdot \delta \mathbf{r}_i = \sum_j \left[\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\mathbf{q}}_j}\right) - \frac{\partial T}{\partial \mathbf{q}_j} - Q_j\right] \delta q_j \tag{4.57}$$

Note: the only restriction on the constraints is that the net virtual work of the constraint forces vanish. (Includes some non-holonomic constraints!)

In the case of holonomic constraints, it is possible to find a set of independent coordinates that obey the constraint conditions.

$$\mathbf{r}_i = \mathbf{r}_i(q_1, \dots q_N, t)$$
$$\mathbf{F}_i = -\nabla_i V(\mathbf{r}_1, \dots \mathbf{r}_N)$$

$$\begin{aligned} \frac{\partial}{\partial q_j} &= \sum_j \frac{\partial \mathbf{r}_i}{\partial q_j} \frac{\partial}{\partial \mathbf{r}_i} \\ &= \sum_i \frac{\partial \mathbf{r}_i}{\partial q_j} \cdot \nabla_i \end{aligned} \tag{4.58}$$

Generalized forces:

$$\begin{aligned} Q_j &= \sum_i \mathbf{F}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \\ &= -\sum_i \frac{\partial \mathbf{r}_i}{\partial q_j} \cdot \nabla_i V \\ &= -\frac{\partial V}{\partial q_j} \end{aligned} \tag{4.59}$$

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial}{\partial q_j}(T - V) = 0 \tag{4.60}$$

If $V = V(\mathbf{r}_1, \dots \mathbf{r}_N)$ as above, then:

$$\frac{\partial V}{\partial \dot{q}_j} = 0$$

and

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0 \tag{4.61}$$

where $L(q, \dot{q}, t) = T(\dot{q}, q) - V(q, t)$

Note:

$$L'(q, \dot{q}, t) = L(q, \dot{q}, t) + \frac{d}{dt}F(q, t) \tag{4.62}$$

$$\frac{d}{dt}\left(\frac{\partial L'}{\partial \dot{q}_i}\right) - \frac{\partial L'}{\partial \dot{q}_i} = \frac{d}{dt}\left[\frac{\partial}{\partial \dot{q}_i}\left(L + \frac{dF}{dt}\right)\right] - \frac{\partial}{\partial q_i}\left[L + \frac{dF}{dt}\right] \tag{4.63}$$

$$\frac{d}{dt}F(q, t) = \sum_i \dot{q}_i \frac{\partial F}{\partial q_i} + \frac{\partial F}{\partial t} \tag{4.64}$$

$$\frac{\partial}{\partial \dot{q}_i}\left(\frac{dF}{dt}\right) = \frac{\partial F}{\partial q_i} \qquad \left(\frac{\partial}{\partial q_i}\right)\frac{d}{dt} = \frac{d}{dt}\left(\frac{\partial}{\partial q_i}\right)$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) + \frac{d}{dt}\left(\frac{\partial F}{\partial q_i}\right) - \frac{\partial L}{\partial q_i} - \left(\frac{\partial}{\partial q_i}\right)\frac{d}{dt}F = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} \tag{4.65}$$

4.4 Velocity-dependent potentials and dissipation functions

Recall:

$$Q_j = \sum_i \mathbf{f}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_i} \tag{4.66}$$

if $\mathbf{F}_i = -\nabla_i v(\mathbf{r}_1, \ldots \mathbf{r}_N)$, and $Q_j = -\frac{\partial v}{\partial q_j}$

If there is a $U(q, \dot{q}, t)$ s.t.

$$Q_j = -\frac{\partial U}{\partial q_j} + \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}_j}\right) \tag{4.67}$$

Then, clearly D'Alembert's principle:

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial}{\partial q_j}T = Q_j = \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}_j}\right) - \frac{\partial U}{\partial q_j} \tag{4.68}$$

or with $L = T - U$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0$$

$U =$ "generalized potential"

$$\begin{aligned}\mathbf{F} &= q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})] \\ &= q[-\nabla\phi - \frac{d\mathbf{A}}{dt} + \nabla(\mathbf{A} \cdot \mathbf{v})]\end{aligned} \tag{4.69}$$

$$\mathbf{E}(\mathbf{r}, t) = -\nabla\phi(\mathbf{r}, t) - \frac{\partial A}{\partial t} \tag{4.70}$$

$$\mathbf{B}(\mathbf{r},t) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r},t) \tag{4.71}$$

$$\begin{aligned}\mathbf{F} =& -\nabla U + \frac{d}{dt}\left(\frac{\partial U}{\partial \mathbf{v}}\right) \\ =& q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})]\end{aligned} \tag{4.72}$$

$$\mathbf{U}(\mathbf{r},t) = q[\phi - \mathbf{A} \cdot \mathbf{v}] \tag{4.73}$$

Proof:

$$\begin{aligned}-\nabla U(\mathbf{r},t) = q[-\nabla\phi + \nabla(\mathbf{A} \cdot \mathbf{v})] \\ \frac{d}{dt}\left(\frac{\partial U}{\partial \mathbf{v}}\right) = -q\frac{d\mathbf{A}}{dt}\end{aligned} \tag{4.74}$$

Where:

$$\nabla(\mathbf{A} \cdot \mathbf{v}) = (\mathbf{A} \cdot \nabla)\mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{A} + \mathbf{A} \times (\nabla \times \mathbf{v}) + \mathbf{v} \times (\nabla \times \mathbf{A})$$

Note:
$\nabla \times \mathbf{r} = 0$, so $\nabla \times \mathbf{v} = 0$ also,

$$\begin{aligned}\frac{\partial}{\partial x}(\mathbf{v}) =& \frac{d}{dt}\frac{\partial}{\partial x}(\mathbf{r}) \\ =& \frac{d}{dt}\hat{x} \\ =& 0\end{aligned} \tag{4.75}$$

$$\nabla(\mathbf{A} \cdot \mathbf{v}) = (\mathbf{v} \cdot \nabla)\mathbf{A} + \mathbf{v} \times (\nabla \times \mathbf{A}) = (\mathbf{v} \cdot \nabla)\mathbf{A} + \mathbf{v} \times \mathbf{B}$$

Note:

$$\begin{aligned}\frac{d\mathbf{A}}{dt} =& \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{A} \\ =& \left(\frac{d\mathbf{A}}{dt} - \frac{\partial \mathbf{A}}{\partial t}\right) + \mathbf{v} \times \mathbf{B}\end{aligned} \tag{4.76}$$

$$\begin{aligned}\mathbf{F} =& -\nabla U + \frac{d}{dt}\left(\frac{\partial U}{\partial \mathbf{v}}\right) \\ =& q\left[-\nabla\phi + \left(\frac{d\mathbf{A}}{dt} - \frac{\partial \mathbf{A}}{\partial t}\right) + \mathbf{v} \times \mathbf{B} - \frac{d\mathbf{A}}{dt}\right] \\ =& q[\mathbf{E} + \mathbf{v} \times \mathbf{B}]\end{aligned} \tag{4.77}$$

4.5 Frictional forces

$$\begin{aligned}F =& \frac{1}{2}\sum_i \mathbf{v}_i \cdot \overleftrightarrow{k} \cdot \mathbf{v}_i \\ =& \frac{1}{2}\sum_i (k_x v_{ix}^2 + k_y v_{iy}^2 + k_z v_{iz}^2)\end{aligned} \tag{4.78}$$

Suppose a force cannot be derived from a scalar potential $U(q,\, \dot{q},\, t)$ by the prescription: $Q_j = -\frac{\partial U}{\partial q_j} + \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}_j}\right)$ for example, the frictional force $F_{fix} = -k_x v_{ix}$. In this case we cannot use Lagrange's equations in their form, but rather in the form:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = Q_j - \left[\frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}_j}\right) - \frac{\partial U}{\partial q_j}\right] = Q_{fi} \tag{4.79}$$

In the case of a frictional force, Q_{fi} can be derived $\mathbf{F}_{fi} = -\nabla_{\mathbf{v}_i} F$
where $F = \frac{1}{2}\sum_i (k_x v_{ix}^2 + k_y v_{iy}^2 + k_z v_{iz}^2)$ (Rayleigh's dissipation function)

Work done on the system = -work done by the system.

Note:

$$\begin{aligned} W_f &= \int \mathbf{F}_f \cdot d\mathbf{r} && (4.80) \\ &= \int \underbrace{-\nabla F \cdot \mathbf{v}}_{-2F} dt \\ &= \int \frac{dW_f}{dt} dt \end{aligned}$$

$$\tag{4.81}$$

$2F =$ the rate of energy dissipation due to friction.

Transforming to generalized coordinates:

recall: $\frac{\partial \mathbf{r}_i}{\partial q_j} = \frac{\partial \mathbf{v}_i}{\partial \dot{q}_j}$

$$\begin{aligned} Q_j &= \sum_i \mathbf{F}_{fi} \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \\ &= \sum_i -\nabla_{\mathbf{v}_i} F \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \\ &= \sum_i -\frac{\partial \mathbf{v}_i}{\partial \dot{q}_j} \cdot \nabla_{\mathbf{v}_i} F \\ &= -\frac{\partial F}{\partial \dot{q}_j} \end{aligned} \tag{4.82}$$

$Q_j = -\frac{\partial F}{\partial \dot{q}_j} =$ the generalized force arising from friction

Derived from $\mathbf{F}_{fi} = -\nabla_{\mathbf{v}_i} F$

The "Lagrange" equations become:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = -\frac{\partial F}{\partial \dot{q}_j} \tag{4.83}$$

Transformation of the kinetic energy to generalized coordinates

$$\begin{aligned}T =& \sum_i \frac{1}{2} m_i v_i^2 \\ =& \sum_i \frac{1}{2} m_i \left(\sum_j \frac{\partial \mathbf{r}_i}{\partial q_j} \dot{q}_j + \frac{\partial \mathbf{r}_i}{\partial t} \right)^2 \\ =& m_o + \sum_j m_j \dot{q}_j + \frac{1}{2} \sum_{j,k} m_{jk} \dot{q}_j \dot{q}_k \\ =& T_o + T_1 + T_2\end{aligned} \tag{4.84}$$

$$m_o = \sum_i \frac{1}{2} m_i \left(\frac{\partial \mathbf{r}_i}{\partial t} \right)^2 \tag{4.85}$$

$$m_j = \sum_i m_i \frac{\partial \mathbf{r}_i}{\partial t} \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \tag{4.86}$$

$$m_{jk} = \sum_i m_i \frac{\partial \mathbf{r}_i}{\partial q_j} \cdot \frac{\partial \mathbf{r}_i}{\partial q_k} \tag{4.87}$$

$$m_o \text{ and } m_j = 0, \text{ if } \frac{\partial \mathbf{r}_i}{\partial t} = 0$$

Problem 23 of Goldstein

$$L = T - V \tag{4.88}$$

$$= \frac{1}{2} m v_z^2 - mgz \tag{4.89}$$

$$F = \frac{1}{2} k v_z^2 \tag{4.90}$$

$$\begin{aligned}Q_z =& - \frac{\partial F}{\partial v_z} \\ =& - k v_z\end{aligned} \tag{4.91}$$

Lagrange's equation:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial v_z} \right) - k v_z \tag{4.92}$$

$$\frac{d}{dt}(m v_z) + mg = -k v_z$$

or

$$\frac{d v_z(t)}{dt} + \left(\frac{k}{m} \right) v_z(t) = -g$$

This is of the form:

$$\frac{dy(t)}{dt} + p(t) y(t) = q(t)$$

or

$$\frac{d}{dt}[\alpha(t)y(t)] = \alpha(t)$$

where:

$$\alpha(t) = e^{\int^t p(t')dt'}$$
$$\frac{d\alpha}{dt} = \alpha(t)p(t)$$

In our case:

$$\begin{aligned}\alpha(t) =& e^{\int^t \frac{k}{m}t'dt'} \\ =& e^{\frac{k}{m}t}\end{aligned} \tag{4.93}$$

$$\begin{aligned}\frac{d}{dt}\left[e^{\frac{k}{m}t}V_z(t)\right] =& \left[\frac{dV_z(t)}{dt} + \frac{k}{m}V_z(t)\right]e^{\frac{k}{m}t} \\ =& -ge^{\frac{k}{m}t}\end{aligned} \tag{4.94}$$

$$\begin{aligned}e^{\frac{k}{m}t}V_z(t) =& \int^t \left(-ge^{\frac{k}{m}t'}\right)dt' \\ =& -\left(\frac{mg}{k}\right)e^{\frac{k}{m}t} + c\end{aligned} \tag{4.95}$$

$$\begin{aligned}V_z(t) =& -\frac{mg}{k} + ce^{-\frac{k}{m}t} \\ =& -\frac{mg}{k}\left[1 - e^{-\frac{k}{m}t}\right]\end{aligned} \tag{4.96}$$

$$\begin{aligned}V_z(0) =& -\frac{mg}{k} + c \\ =& 0\end{aligned} \tag{4.97}$$

$$c = \frac{mg}{k} \tag{4.98}$$

$$\frac{dV_z}{dt} = 0 \qquad\qquad t^* = \infty$$

$$\begin{aligned}V_z^* =& \lim_{t\to\infty} V_z(t) \\ =& -\frac{mg}{k}\end{aligned} \tag{4.99}$$

$$\begin{aligned}\lim_{x\to 0}\frac{1-e^{xt}}{x} =& \lim_{x\to 0} -te^x \\ =& -t\end{aligned} \qquad\qquad x = -\frac{k}{m}$$

Note:

$$\lim_{\frac{k}{m}\to 0} V_z(t) = -gt \tag{4.100}$$

Chapter 5

Variational Principles

Particle sliding down a movable wedge (frictionless)

$$
\begin{aligned}
x_m &= s \cdot \cos\theta + x & \dot{x}_m &= \dot{s} \cdot \cos\theta + \dot{x} \\
y_m &= -\sin\theta & \dot{y}_m &= -\dot{s} \cdot \sin\theta \\
x_M &= x & \dot{x}_M &= \dot{x} \\
y_M &= 0 & \dot{y}_M &= 0
\end{aligned}
$$

$$
\begin{aligned}
T &= \frac{1}{2}m(\dot{x}_m^2 + \dot{y}_m^2) + \frac{1}{2}M(\dot{x}_M^2 + \dot{y}_M^2) \\
&= \frac{1}{2}m(\dot{s}^2 + 2\dot{x}\dot{s} \cdot \cos\theta + \dot{x}^2) + \frac{1}{2}M\dot{x}^2
\end{aligned} \tag{5.1}
$$

$$
\begin{aligned}
V =& mgy \\
=& - mg \cdot \sin\theta
\end{aligned} \tag{5.2}
$$

$$
L = \frac{1}{2}m(\dot{s}^2 + 2\dot{x}\dot{s} \cdot \cos\theta + \dot{x}^2) + \frac{1}{2}M\dot{x}^2 + mgs \cdot \sin\theta \tag{5.3}
$$

$$
\begin{aligned}
&\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{s}}\right) - \frac{\partial L}{\partial s} = 0 & &\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0 \\
&\frac{\partial L}{\partial s} = mg \cdot \sin\theta & &\frac{\partial L}{\partial x} = 0 \\
&\frac{\partial L}{\partial \dot{s}} = m\dot{s} + m\dot{x} \cdot \cos\theta & &\frac{\partial L}{\partial \dot{x}} = (m+M)\dot{x} + m\dot{s} \cdot \cos\theta \\
&\frac{d}{dt}[m\dot{s} + m\dot{x} \cdot \cos\theta] = mg \cdot \sin\theta & &\frac{d}{dt}[\underbrace{(m+M)\dot{x} + m\dot{s} \cdot \cos\theta}_{\text{constant of motion}}] = 0
\end{aligned}
$$

1. $\ddot{s}(m) + \ddot{x}(m \cdot \cos\theta) = mg \cdot \sin\theta$

2. $\ddot{s}(m \cdot \cos\theta) + \ddot{x}(m+M) = 0$

$(1.) - \frac{(2.)}{\cos\theta}$ gives:

$$\ddot{x}\left[m\cdot\cos\theta - \frac{(m+M)}{\cos\theta}\right] = mg\cdot\sin\theta \tag{5.4}$$

or

$$\begin{aligned}\ddot{x} =& mg\cdot\sin\theta\cdot\left[\frac{\cos\theta}{m\cos^2\theta-(m+M)}\right] \\ =& A_x\end{aligned} \tag{5.5}$$

$$x(t) = x_o + \dot{x}_o t + \frac{1}{2}A_x t^2 \tag{5.6}$$

$(1.) - \frac{m\cdot\cos\theta}{(m+M)}(2.)$ gives:

$$\ddot{s}\left[m - \frac{(m\cdot\cos\theta)^2}{(m+M)}\right] = mg\cdot\sin\theta \tag{5.7}$$

or

$$\begin{aligned}\ddot{s} =& mg\cdot\sin\theta\cdot\left[\frac{(m+M)}{m(m+M)-m^2\cdot\cos^2\theta}\right] \\ =& A_s\end{aligned} \tag{5.8}$$

$$s(t) = s_o + \dot{s}_o t + \frac{1}{2}A_s t^2 \tag{5.9}$$

5.1 Hamilton's Principle

A monogenic system is one where all forces (except for those of constraint) are derivable from a generalized scalar potential $U(q, \dot{q}, t)$.

If the scalar potential is only a function of the coordinates, $U(q)$, a monogenic system is also conservative. Hamilton's Principle (The principle of least action)

Fundamental postulate of classical mechanics for monogenic systems under holonomic constraints to replace Newton's equations of motion.

For monogenic systems, the classical motion of a system (i.e., it's path through phase space) between time t_a and t_b is the one for which the action integral:

$$S(a,b) = \int_{t_a}^{t_b} L(q,\dot{q},t)dt \tag{5.10}$$

$$L = T - U \tag{5.11}$$

has a stationary value, that is to say $\delta S = 0$, which leads to the Lagrange equations: $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$, and the generalized forces are:

$$Q_j = \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}}\right) - \frac{\partial U}{\partial q} \tag{5.12}$$

5.2 Comments about Hamilton's Principle

$\delta S = 0$ poses no restrictions to the particular set of generalized coordinates used to represent the motion of the system, and therefore are automatical, invariant to transformations* between sets of generalized coordinates.

*Transformations with $det(J) \neq 0$, i.e. that span the same space.

Note: Hamilton's Principle takes the form of an un-constrained variation of the action integral.
If the system constraints are holonomic, i.e. can be written as :

$$f_\alpha(q_1, q_2, \dots q_N) = 0$$
$$\alpha = 1, \dots K$$

Then a set of generalized coordinates can always be found, $q_1', q_2' \dots q_{N-K}'$, that satisfy the constraint conditions, in which case Hamilton's Principle is both a necessary and sufficient condition for Lagrange's equations.

If nonholonomic constraints are present such that a set of generalized coordinates cannot be defined that satisfy the constraints, sometimes these constraints can be introduced through a constrained variation of the action integral with the method of Lagrange multipliers.

Suppose we consider a more general form of constraint, formally a type of nonholonomic constraint, called semi-holonomic:

$$f_\alpha(q_1, q_2, \dots q_N, \dot{q}_1, \dot{q}_2, \dots \dot{q}_N, t) = 0$$
$$\alpha = 1, \dots K$$

Consider the constrained variation of the action:

$$\delta \int \left(L(q, \dot{q}, t) + \sum_{\alpha<1}^{k} \lambda_\alpha(q, \dot{q}, t) f_\alpha(q, \dot{q}) \right) dt = 0 \tag{5.13}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) - \frac{\partial L}{\partial q_k} + \frac{d}{dt}\left[\frac{\partial}{\partial \dot{q}_k}\left(\sum_\alpha \lambda_\alpha f_\alpha\right)\right] - \frac{\partial}{\partial q_k}\left(\sum_\alpha \lambda_\alpha f_\alpha\right) = 0 \tag{5.14}$$

or

$$Q_k' = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) - \frac{\partial L}{\partial q_k} \tag{5.15}$$

where

$$Q_k' = \frac{\partial}{\partial q_k}\left(\sum_\alpha \lambda_\alpha f_\alpha\right) - \frac{d}{dt}\left[\frac{\partial}{\partial \dot{q}_k}\left(\sum_\alpha \lambda_\alpha f_\alpha\right)\right] \tag{5.16}$$

if the generalized force of constraint, in terms of the yet-to-be-determined Lagrange multipliers λ_α. So here, the forces of constraint will be supplied as part of the solution to the problem!

By solving explicitly for the constraint forces, there is no need to try and find a generalized set of coordinates (which cannot be done for semi-holonomic constraints).

Expanding out the expression for Q_k we obtain:

$$Q_k' = \sum_\alpha \lambda_\alpha \left[\frac{\partial f_\alpha}{\partial q_k} - \frac{d}{dt}\left(\frac{\partial f_\alpha}{\partial \dot{q}_k}\right)\right] + \sum_\alpha \left[\frac{\partial \lambda_\alpha}{\partial q_k} - \frac{d}{dt}\left(\frac{\partial \lambda_\alpha}{\partial \dot{q}_k}\right)\right] f_\alpha - \sum_\alpha \left[\frac{\partial \lambda_\alpha}{\partial \dot{q}_k}\frac{df_\alpha}{dt} + \frac{d\lambda_\alpha}{dt}\frac{\partial f_\alpha}{\partial \dot{q}_k}\right] \tag{5.17}$$

Note, in the case of the semi-holonomic constraint condition:

$$f_\alpha(q_1, \ldots q_N, \dot{q}_1, \ldots \dot{q}_N) = 0$$

which must be imposed in order to solve for the λ_α, also implies that $\frac{df_\alpha}{dt} = 0$. Imposition of these conditions on Q'_k leads to:

$$Q'_k = \sum_\alpha \lambda_\alpha \left[\frac{\partial f_\alpha}{\partial q_k} \frac{d}{dt} \left(\frac{\partial f_\alpha}{\partial \dot{q}_k} \right) \right] - \frac{d\lambda_\alpha}{dt} \frac{\partial f_\alpha}{\partial \dot{q}_k} \tag{5.18}$$

which is the same result we would have obtained if we assumed from the start that $\lambda_\alpha = \lambda_\alpha(t)$ only. Note further that if the f_α were actually holonomic constraints, $f_\alpha(q_1, \ldots q_N) = 0$,

$$Q'_k = \sum_\alpha \lambda_\alpha \frac{\partial f_\alpha}{\partial q_k} \tag{5.19}$$

which is often seen in other texts.

Example of a hoop on a wedge

$$M = \text{mass of hoop}$$

$$T = \frac{1}{2} M v^2 + \frac{1}{2} I \omega^2 \tag{5.20}$$

$$v = \dot{x} \tag{5.21}$$

$$I = M r^2 \tag{5.22}$$

$$\omega = \dot{\theta} \tag{5.23}$$

$$T = \frac{1}{2} M \dot{x}^2 + \frac{1}{2} M r^2 \dot{\theta}^2 \tag{5.24}$$

$$\begin{aligned} V &= mgy \\ &= Mg(\ell - x) \sin\phi \end{aligned} \tag{5.25}$$

$$L = \frac{1}{2} M \dot{x}^2 + \frac{1}{2} M r^2 \dot{\theta}^2 - Mg(\ell - x) \sin\phi \tag{5.26}$$

Unconstrained variation of the action leads to:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0 \qquad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = 0$$

$$\frac{d}{dt}(M\dot{x}) - Mg \cdot \sin\phi = 0 \qquad \frac{d}{dt}(Mr^2\dot{\theta}) - 0 = 0$$

$$\ddot{x} = g \cdot \sin\phi \qquad \ddot{\theta} = 0$$

$$x(t) = x_o + \dot{x}_o t + \frac{1}{2} g \cdot \sin\phi \cdot t^2 \qquad \theta(t) = \theta_o + \dot{\theta}_o \cdot t$$

If starting at rest at top of wedge $(x_o = 0, \dot{x}_o = 0)$ the time it would take to go down would be:

$$x(t_f) = \ell = \frac{1}{2} g \cdot \sin\phi \cdot t_f^2 \tag{5.27}$$

$$t_f = \sqrt{\frac{2\ell}{g \cdot \sin\phi}}$$

Note, t_f does not depend on θ_o or $\dot{\theta}_o$. If $\theta_o = 0$ and $\dot{\theta}_o = 0$, then $\theta(t) = 0$, and the hoop completely slips down the wedge.

Consider now the constraint the hoop must roll down the wedge without slipping. The constraint condition is that $rd\theta = dx$, or $r\dot{\theta} = \dot{x}$, hence:

$$f_1 = r\dot{\theta} - \dot{x} = 0$$

The constrained variation $\delta\{\int(L + \lambda_1 f_1)dt\} = 0$ gives:

$$\begin{aligned} Q'_x &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial \dot{x}} \\ Q'_x &= \lambda_1 \left[\frac{\partial f_1}{\partial x} - \frac{d}{dt}\left(\frac{\partial f_1}{\partial \dot{x}}\right)\right] \\ &= -\dot{\lambda}_1 \frac{\partial f_1}{\partial \dot{x}} \\ &= 0 - \dot{\lambda}_1(-1) = \dot{\lambda}_1 \end{aligned}$$

$$\begin{aligned} Q'_\theta &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \dot{\theta}} \\ Q'_\theta &= \lambda_1 \left[\frac{\partial f_1}{\partial \theta} - \frac{d}{dt}\left(\frac{\partial f_1}{\partial \dot{\theta}}\right)\right] \\ &= -\dot{\lambda}_1 \frac{\partial f_1}{\partial \dot{\theta}} \\ &= 0 - \dot{\lambda}_1 r = -\dot{\lambda}_1 r \end{aligned}$$

$$r\ddot{\theta} - \ddot{x} = 0 \tag{5.28}$$

$$\frac{d}{dt}(M\dot{x}) - Mg \cdot \sin\phi = \dot{\lambda}_1 \tag{5.29}$$

$$\frac{d}{dt}(Mr^2\dot{\theta}) = -\dot{\lambda}_1 r \tag{5.30}$$

Solving for $\ddot{x}$, $\ddot{\theta}$ and $\dot{\lambda}$ we obtain:

$$\begin{aligned} Mr^2\ddot{\theta} =& -\dot{\lambda}_1 r \\ =& Mr\ddot{x} \end{aligned} \tag{5.31}$$

$$\tag{5.32}$$

or

$$\begin{aligned} M\ddot{x} =& -\dot{\lambda}_1 \\ =& \dot{\lambda}_1 Mg \cdot \sin\phi \end{aligned} \tag{5.33}$$

$$\tag{5.34}$$

or

$$\dot{\lambda}_1 = \frac{-Mg \cdot \sin\phi}{2} \tag{5.35}$$

$$\ddot{x} = \frac{g \cdot \sin\phi}{2} \tag{5.36}$$

$\frac{1}{2}$ the acceleration with slipping

$$\ddot{\theta} = \frac{g \cdot \sin\phi}{2r} \tag{5.37}$$

$$t_f = \sqrt{\frac{4\ell}{g \cdot \sin\phi}} \tag{5.38}$$

Note: we "pretended" in this problem we had a semi-holonomic constraint

$$f_\alpha = r\dot{\theta} - \dot{x} = 0 = f_\alpha(\dot{x}, \dot{\theta})$$

but really we could have stated this as a holonomic constraint

$$f_\alpha = r\theta - x = 0 = f_\alpha(x, \theta)$$

in which case the Q'_x's are in holonomic form:

$$Q'_x = \lambda_1 \frac{\partial f_\alpha}{\partial x} = -\lambda_1 \qquad Q'_\theta = \lambda_1 \frac{\partial f_\alpha}{\partial \theta} = \lambda_1 r$$

Carrying through, we again obtain the equations of motion.

$$\ddot{x} = \frac{g \cdot \sin\phi}{2} \qquad \ddot{\theta} = \frac{g \cdot \sin\phi}{2r}$$

but λ is given by:

$$\lambda = Mg\frac{\sin\phi}{2} \tag{5.39}$$

In this case, λ amounts to a frictional force of the non-slipping constraint, $\frac{Mg \cdot \sin\phi}{2}$, that is $\frac{1}{2}$ the magnitude of gravitational force along the wedge $-\frac{d}{dy}(Mgy) = -Mg \cdot \sin\phi$, and in the opposite direction.

The "first integral" of Lagrange's equations
Note:

$$\frac{d}{dt}\left[L(q, \dot{q}, t) - \sum_k \dot{q}_k \frac{\partial L}{\partial \dot{q}_k}\right]$$

$$\begin{aligned} &= \frac{\partial L}{\partial t} + \sum_k \dot{q}_k \frac{\partial L}{\partial q_k} + \sum_k \ddot{q}_k \frac{\partial L}{\partial \dot{q}_k} - \sum_k \ddot{q}_k \frac{\partial L}{\partial \dot{q}_k} - \sum_k \dot{q}_k \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) \\ &= \frac{\partial L}{\partial t} - \sum_k \dot{q}_k \left[\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) - \frac{\partial L}{\partial q_k}\right] \end{aligned} \tag{5.40}$$

Hence, if $\frac{\partial L}{\partial t} = 0$, then

$$\sum_k \dot{q}_k \left[\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) - \frac{\partial L}{\partial q_k}\right] = 0 \tag{5.41}$$

If the Lagrange equations $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) - \frac{\partial L}{\partial q_k} = 0$ are satisfied, this gives the first integral equation:

$$\frac{d}{dt}\left[L(q, \dot{q}, t) - \sum_k \dot{q}_k \frac{\partial L}{\partial \dot{q}_k}\right] = \frac{\partial L}{\partial t} \tag{5.42}$$

5.3 Conservation Theorems and Symmetry

We define a generalized momentum as $P_j \equiv \frac{\partial L}{\partial \dot{q}_j}$ that is said to be conjugate to q_j. Sometimes this is called the canonical momentum.

It is clear by the first integral equation that if $\frac{\partial L}{\partial t} = 0$, then:

$$-\left[\sum_k \dot{q}_k \frac{\partial L}{\partial \dot{q}_k} - L(q, \dot{q}, t)\right] = \text{ constant “energy function”}$$

$$\frac{d}{dt} h(q_1, \dots q_N, \dot{q}_1 \dots \dot{q}_N, t) = -\frac{\partial L}{\partial t}$$

If there is an “ignorable” coordinate in that $\frac{\partial L}{\partial q_k} = 0$, then clearly:

$$\frac{d}{d}\left(\frac{\partial L}{\partial \dot{q}_k}\right) = 0 = \frac{d}{dt} P_k$$

hence $P_k =$constant

Also more generally if:

$$\sum_k W_k \frac{\partial L}{\partial q_k} = 0, \text{ where } W_k \neq W_k(t)$$

$$\text{then } \sum_k W_k P_k = \text{ constant}$$

Symmetry: Finally note that time t is “reversible” in the equations of motion: reversing the velocities $\dot{q}(t)$ sends the trajectory backwards along the same path.

Chapter 6

Central Potential and More

6.1 Galilean Transformation

A Galilean transformation is one such that:

$$\mathbf{r}(t) = \mathbf{r}'(t') + \mathbf{v} \cdot t' = \mathbf{r}'(t) + \mathbf{v} \cdot t$$

since $t = t'$ and relates two reference frames to one another, where the $\mathbf{r}'$ frame moves with constant velocity relative the $\mathbf{r}$ frame.

A fundamental assumption of classical mechanics (that breaks down in relativistic mechanics) is that the classical equations of motion are invariant to Galilean transformation.

6.2 Kinetic Energy

The kinetic energy of a particle is:

$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \qquad \text{Cartesian} \qquad (6.1)$$

$$= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin\theta \cdot \dot{\phi}^2) \qquad \text{Spherical} \qquad (6.2)$$

$$= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2 + \dot{z}^2) \qquad \text{Cylindrical} \qquad (6.3)$$

6.3 Motion in 1-Dimension

6.3.1 Cartesian Coordinates

$$L = \frac{1}{2}m\dot{x}^2 - U(x) \tag{6.4}$$

$$\frac{d}{dt}(m\dot{x}) - \frac{\partial L}{\partial x} = 0 \tag{6.5}$$

or

$$-\frac{d}{dt}\left[L - \dot{x}\frac{\partial L}{\partial \dot{x}}\right] = 0 \tag{6.6}$$

$$-\left[\frac{1}{2}m\dot{x}^2 - U(x) - m\dot{x}^2\right] = \frac{1}{2}m\dot{x}^2 + U(x) \tag{6.7}$$
$$= E = \text{ constant}$$

$$\dot{x} = \frac{dx}{dt} = \sqrt{\frac{2}{m}(E - U(x))} \tag{6.8}$$

$$dt = \frac{dx}{\sqrt{\frac{2}{m}(E - U(x))}} \qquad t = \int \frac{dx}{\sqrt{\frac{2}{m}(E - U(x))}} \cdot c$$

Since $E = T + U$ and $T \geq 0$ and $E \geq U$. When $E = U(x_E)T = 0$, so the x_E are “turning points.”

Calculating the period $T(E)$ between the turing points $x_1(E)$ and $x_2(E)$:

$$T(E) = \int_{x_1(E)}^{x_2(E)} dt + \int_{x_2(E)}^{x_1(E)} (-dt) \tag{6.9}$$
$$= 2\int_{x_1(E)}^{x_2(E)} dt$$
$$= 2\int_{x_1(E)}^{x_2(E)} \frac{dx}{\sqrt{\frac{2}{m}(E - U(x))}}$$

6.3.2 Generalized Coordinates

$$L = \frac{1}{2}m\dot{x}^2 - U(x) \tag{6.10}$$
$$= T(\dot{x}) - U(x)$$

in general, $T = T_o(q) + T_1(q, \dot{q}) + T_2(q, \dot{q})$ if $x = x(q)$ and not $x = x(q, t)$, then:

$$T(q, \dot{q}) = T_2(q, \dot{q}) \tag{6.11}$$
$$= \frac{1}{2}ma(q)\dot{q}^2$$

$$L = \frac{1}{2}m \cdot a(q) \cdot \dot{q}^2 - U(q) \tag{6.12}$$

$$E = \dot{q}\frac{\partial L}{\partial \dot{q}} - L \tag{6.13}$$
$$= \frac{1}{2}ma(q)\dot{q}^2 + U(q)$$

$$\sqrt{\frac{2}{m} \cdot a(q)\left[E - U(q)\right]} = \dot{q} = \frac{dq}{dt} \tag{6.14}$$

$$dt = \frac{dq}{\sqrt{\frac{2}{m} \cdot a(q)\left[E - U(q)\right]}} \qquad t = \sqrt{\frac{m}{2}} \int \frac{dq}{\sqrt{a(q)\left[E - U(q)\right]}} + C$$

$$T(E) = 2\sqrt{\frac{M}{2}} \int_{x_1(E)}^{x_2(E)} \frac{dq}{\sqrt{a(q)\left[E - U(x)\right]}} \tag{6.15}$$

6.4 Classical Viral Theorem

(for central forces)

Consider $G = \sum_i \mathbf{p}_i \cdot \mathbf{r}_i$ for a system of particles:

$$\frac{dG}{dt} = \sum_i \dot{\mathbf{p}}_i \cdot \mathbf{r}_i + \sum_i \mathbf{p}_i \cdot \dot{\mathbf{r}}_i$$

from $\frac{d}{dt}\mathbf{p}_i = \mathbf{F}_i$

$$\begin{aligned}\frac{dG}{dt} &= \sum_i \mathbf{F}_i \cdot \mathbf{r}_i + \sum_i \mathbf{m}_i \cdot \dot{\mathbf{r}}_i^2 \\ &= \sum_i \mathbf{F}_i \cdot \mathbf{r}_i + 2T\end{aligned}$$

Consider:

$$\langle A \rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau A(t) dt \tag{6.16}$$

$$\begin{aligned}\left\langle \frac{dG}{dt} \right\rangle &= \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \frac{dG}{dt} dt \\ &= \frac{1}{\tau} \lim_{\tau \to \infty} \left[G(\tau) - G(0)\right] \\ &= 0, \text{ when } \lim_{\tau \to \infty} G(\tau) < \text{constant}\end{aligned} \tag{6.17}$$

In this case,

$$\left\langle \frac{dG}{dt} \right\rangle = 0 = \langle 2T \rangle + \left\langle \sum_i \mathbf{F}_i \cdot \mathbf{r}_i \right\rangle$$

or

$$2\langle T \rangle = -\left\langle \sum_i \mathbf{F}_i \cdot \mathbf{r}_i \right\rangle \qquad \text{Viral theorem} \tag{6.18}$$

If $\mathbf{F}_i = -\nabla_i V(\mathbf{r}_1, \ldots \mathbf{r}_N)$ and $V(\mathbf{r}_1, \ldots \mathbf{r}_N)$ is a homogeneous function of degree $n+1$ in the $\mathbf{r}_i$,

$$\begin{aligned}2\langle T \rangle &= \left\langle \sum_i \nabla_i V(\mathbf{r}_1, \ldots \mathbf{r}_N) \cdot \mathbf{r}_i \right\rangle \\ &= (n+1)\langle V \rangle\end{aligned} \tag{6.19}$$

For a central force:

$$V(r) = ar^{n+1} \qquad F_r = -(n+1)ar^n \sim r^n$$

$$2\langle T \rangle = (n+1)\langle V \rangle \text{ or } \langle T \rangle = \frac{(n+1)}{2}\langle V \rangle$$

6.5 Central Force Problem

A monogenic system of 2 mass particles interacting via $V(\mathbf{r}_2 - \mathbf{r}_1)$, we have:

$$\begin{aligned} L =& T(\dot{\mathbf{R}}, \dot{\mathbf{r}}) - U(\mathbf{r}, \dot{\mathbf{r}}, \ldots) \\ =& \frac{1}{2} M \dot{R}^2 + \frac{1}{2}\mu \dot{r}^2 - U(\mathbf{r}, \dot{\mathbf{r}}, \ldots) \end{aligned} \tag{6.20}$$

$$\mathbf{R} \equiv \frac{1}{M}\sum_i m_i \mathbf{r}_i = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}\,, \qquad \mathbf{r} \equiv \mathbf{r}_2 - \mathbf{r}_1 \tag{6.21}$$

$$M = \sum_i m_i = m_1 + m_2$$

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$$

or

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{R}}}\right) - \frac{\partial L}{\partial \mathbf{R}} = M\ddot{\mathbf{R}} = 0 \tag{6.22}$$

$$\mathbf{R}(t) = \mathbf{R}_o + \dot{\mathbf{R}}_o t \tag{6.23}$$

For $V = V(\mathbf{r})$:

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{r}}}\right) - \frac{\partial L}{\partial \mathbf{r}} =& \mu\ddot{\mathbf{r}} - \frac{\partial V}{\partial \mathbf{r}} \\ =& \mu\ddot{\mathbf{r}} - \left(\frac{1}{r}\frac{dV}{dr}\right)\mathbf{r} \end{aligned} \tag{6.24}$$

For $V = V(r)$ we have the following constants of motion:

$M\dot{\mathbf{R}} = \text{constant}$	(total linear momentum)
$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \text{constant}$	(angular momentum about the center of mass)

$$L = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2) - V(r) \tag{6.25}$$

Since $\mathbf{L}$ is conserved (a constant), and $\mathbf{L} \cdot \mathbf{r} = 0$, ($\mathbf{L} \perp \mathbf{r}$) motion must occur in a plane.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = \frac{d}{dt}\underbrace{(\mu r^2 \dot{\theta})}_{P_\theta} - 0 = 0 \tag{6.26}$$

$$\mu r^2 \ddot{\theta} = 0 \tag{6.27}$$

$$I\omega^2 = \dot{P}_\theta \tag{6.28}$$

1. $\mu r^2\dot{\theta} = P_\theta = \ell$ (6.29)
constant (angular momentum)

(Kepler's 2^{nd} Law)

Note: $\mu r^2\ddot{\theta} = 0$ implies also $\underbrace{\left[\frac{1}{2}r\cdot(r\dot{\theta})\right]}_{\text{(sectorial velocity)}} = \text{constant}$

$$2.\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}}\right) - \frac{\partial L}{\partial \dot{r}} = \frac{d}{dt}(\mu\dot{r}) - \mu r\dot{\theta}^2 + \underbrace{\frac{\partial V}{\partial r}}_{\frac{dV}{dr}} = 0 \tag{6.30}$$

$$\ell = 2\mu\left[\frac{dA}{dt}\right] \tag{6.31}$$

$$\frac{dA}{dt} = \text{constant} \tag{6.32}$$

$$\mu\ddot{r} - \frac{\ell^2}{\mu r^3} = -\frac{dV}{dr} \qquad \mu\ddot{r} = -\frac{dV}{dr}\left[V + \frac{1}{2\mu}\left(\frac{\ell}{r}\right)^2\right]$$

Multiply both sides by $\frac{dr}{dt}$, we obtain:

$$\begin{aligned}\mu\ddot{r}\cdot\dot{r} =& \frac{d}{dt}\left(\frac{1}{2}\mu\dot{r}^2\right) \\ =& -\frac{dr}{dt}\frac{d}{dr}\left[V + \frac{1}{2\mu}\left(\frac{\ell}{r}\right)^2\right] \\ =& -\frac{d}{dt}\left[V + \frac{1}{2\mu}\left(\frac{\ell}{r}\right)^2\right]\end{aligned} \tag{6.33}$$

Combining, we obtain the conservation of the energy function (which we knew should be!)

$$\frac{d}{dt}\left[\frac{1}{2}\mu\dot{r}^2 + \frac{1}{2\mu}\left(\frac{\ell}{r}\right)^2 + V\right] = 0 \tag{6.34}$$

or

$$\frac{1}{2}\mu\dot{r}^2 + \frac{1}{2\mu}\left(\frac{\ell}{r}\right)^2 + V = E = \text{ constant} \tag{6.35}$$

Note: this is 1^{st} integral.

$$\dot{\theta}\cdot\mu r^2\dot{\theta} + \dot{r}\mu\dot{r} - \frac{1}{2}\mu r^2\dot{\theta}^2 - \frac{1}{2}\mu\dot{r}^2 + V(r)$$

We begin with the first integral 6.35, since it does not couple r and θ. Solving for $\dot{r}$:

$$\dot{r} = \sqrt{\frac{2}{\mu}(E \underbrace{-V(r) - \frac{\ell^2}{2\mu r^2}}_{-V'(r)})} = \frac{dr}{dt} \tag{6.36}$$

$$V'(r) = V + \frac{\ell^2}{2\mu r^2}$$

$$dt = \frac{dr}{\sqrt{\frac{2}{\mu}\left(E - V(r) - \frac{\ell^2}{2\mu r^2}\right)}} \tag{6.37}$$

$$\text{let } r(t_o) \equiv r_o$$

$$\text{then, } V'(r) = V(r) + \frac{\ell^2}{2\mu r^2}$$

$$t(r) = \int_{r_o}^{r} \frac{dr}{\sqrt{\frac{2}{\mu}\left(E - V(r) - \frac{\ell^2}{2\mu r^2}\right)}} \tag{6.38}$$

$$= \int_{o}^{r} \frac{dr}{\sqrt{\frac{2}{\mu}(E - V'(r))}}$$

Solving for $t(r)$ and inverting gives $r(t)$, then first integral $\mu r\dot{\theta} = \ell = \mu r \frac{d\theta}{dt}$ gives:

$$\theta(t) = \ell \int_0^t \frac{dt}{\mu r^2(t)} + \theta_o \tag{6.39}$$

Note, this is equivalent to the problem of a particle of mass μ moving under the influence of an effective potential:

$$E = \frac{1}{2}\mu\dot{r}^2 + V'(r) \tag{6.40}$$

Example:

$$V'(r) = V(r) + \frac{\ell^2}{2\mu r^2}$$

with

$$F_r' = -\frac{dV}{dr} + \underbrace{\frac{\ell^2}{\mu r^3}}_{\text{centrifugal force}} \tag{6.41}$$

$$E \geq V' \geq V$$

$$V = -\frac{k}{r} \tag{6.42}$$

$$f = -\frac{k}{r^2} \tag{6.43}$$

(gravitational electrostatic)

Sometimes we are interested not necessarily in $r(t)$ and $\theta(t)$, but rather on $r(\theta)$ or $\theta(r)$ or some other relation between r and θ that describe to orbit. Recall:

$$\frac{d\theta}{dt} = \frac{\ell}{\mu r^2} \tag{6.44}$$

$$\frac{dr}{dt} = \sqrt{\frac{2}{\mu}\left(E - V - \frac{\ell^2}{2\mu r^2}\right)} \tag{6.45}$$

$$\frac{dr}{dt} = \frac{d\theta}{dt}\left(\frac{dr}{d\theta}\right) \qquad \frac{dr}{dt} = \frac{\ell}{\mu r^2}\left(\frac{dr}{d\theta}\right) \tag{6.46}$$

$$d\theta \cdot \frac{\mu r^2}{\ell} = dt = \frac{dr}{\sqrt{\frac{2}{\mu}\left(E - V - \frac{\ell^2}{2\mu r^2}\right)}} \tag{6.47}$$

$$d\theta = \frac{\ell \cdot dr}{\mu r^2 \sqrt{\frac{2}{\mu}\left(E - V - \frac{\ell^2}{2\mu r^2}\right)}} \tag{6.48}$$

$$\theta = \int_{r_o}^{r} \frac{dr}{r^2\sqrt{\frac{2\mu E}{\ell^2} - \frac{2\mu V}{\ell^2} - \frac{1}{r^2}}} + \theta_o \tag{6.49}$$

Indroducing a sometimes useful transformation $u = \frac{1}{r}$:

$$\theta = \theta_o - \int_{u_o}^{u} \frac{du}{\sqrt{\frac{2\mu(E-V)}{\ell^2} - u^2}} \tag{6.50}$$

This can be solved for many cases when:

"power law" of force

$$V = a r^{n+1} \tag{6.51}$$

$$F_r = (n+1) a r^n \tag{6.52}$$

$n = 1, -2, -3$ (trigonometric) and $n = 5, 3, 0, -4, -5, -7$ (elliptic)

6.6 Conditions for Closed Orbits

$$V'(r) = V(r) + \frac{\ell^2}{2\mu r^2} \tag{6.53}$$

For circular orbit:

$$E = V(r_o) + \frac{\ell^2}{2\mu r_o^2} + \frac{1}{2}\mu \dot{r}^2 \tag{6.54}$$

$$\begin{aligned} -\frac{dV'}{dr}\bigg|_{r_o} = 0 &= f'(r_o) \\ &= f(r_o) + \frac{\ell^2}{\mu r_o^3} \end{aligned}$$

for circular orbit, equivalent to $f(r_o) = -\frac{\ell^2}{\mu r_o^3}$

$$\text{if} \quad \frac{d^2V'}{dr^2}\bigg|_{r_o} \begin{aligned} &> 0 \quad \text{(stable orbit)} \\ &< 0 \quad \text{(unstable orbit)} \end{aligned}$$

$$-\frac{d^2V'}{dr^2}\bigg|_{r_o} = \frac{df}{dr}\bigg|_{r_o} - \frac{3\ell^2}{\mu r_o^4}$$

For a stable orbit:

$$\frac{df}{dr} < -\frac{3}{r_o} f(r_o)$$

or:

$$\frac{1}{(\frac{1}{r_o})} \frac{a}{f(r_o)} \left(\frac{df}{dr}\right)\bigg|_{r_o} = \frac{d\ln f}{d\ln r}\bigg|_{r_o} > -3$$

(assume $f(r_o) < 0$)

If $f = -kr^n$, a stable orbit requires $n > -3$ if $k > 0$, or $n > 0$ for $k < 0$.

For small perturbations about stable circular orbits:

$$U \equiv \frac{1}{r} = U_o + a\cos\beta\theta$$

Condition for closed orbits(eventually retraces itself), and we have:

$$\frac{d\ln f}{d\ln r} = \beta^2 - 3 \qquad\qquad f(r) = -\frac{k}{r^{3-\beta^2}} \tag{6.55}$$

were β is a rational number.

It turns out, that for arbitrary perturbations (not only small ones), stable closed orbits are possible only for $\beta^2 = 2$ and $\beta^2 = 4$. This was proved by Bertrand.

6.7 Bertrand's Theorem

The only central forces that result in closed orbits for all bound particles are for:

$$f(r) = \frac{-k}{r^3 - \beta^2} \tag{6.56}$$

where:

1. $\beta^2 = 1$ and $f(r) = \frac{-k}{r^2}$ (inverse square law)
2. $\beta^2 = 4$ and $f(r) = -k \cdot r$ (Hooke's law)

6.8 The Kepler Problem

$$V = \frac{-k}{r} \qquad\qquad \mathbf{F} = \frac{-k}{r^2}\left(\frac{\mathbf{r}}{r}\right)$$

The equation for the orbit in the Kepler problem:

$$\theta = \theta' - \int \frac{du}{\sqrt{\frac{2\mu}{\ell^2}\left[E - V\left(\frac{1}{u}\right)\right] - u^2}} \qquad \text{(indefinite integral)} \tag{6.57}$$

$$= \theta' - \int \frac{du}{\sqrt{\frac{2\mu}{\ell^2}[E + ku] - u^2}} \qquad V = -k \cdot u$$

Note:

$$\int \frac{du}{\sqrt{\alpha + \beta u + \gamma u^2}} = -\frac{1}{\sqrt{-\gamma}} \arccos\left[-\frac{\beta + 2\gamma u}{\sqrt{q}}\right] \tag{6.58}$$

where $q \equiv \beta^2 - 4\alpha\gamma$
let:

$$\alpha \equiv \frac{2\mu E}{\ell^2} \qquad \beta = \frac{2\mu k}{l^2} \qquad \gamma = -1$$

$$q = \left(\frac{2\mu k}{\ell^2}\right)^2 \left(1 + \frac{2E\ell^2}{\mu k^2}\right) \tag{6.59}$$

Note: $\cos(a) = \cos(-a)$, thus $\arccos$ can give $\pm$

$$\theta = \theta' - \arccos\left[\frac{\left(\frac{\ell^2 U}{\mu k - 1}\right)}{\sqrt{1 + \frac{2E\ell^2}{\mu k^2}}}\right] \tag{6.60}$$

$$\sqrt{1 + \frac{2E\ell^2}{\mu k^2}} = e$$

$$-\cos(\theta - \theta') = \frac{\left(1 - \frac{\ell^2 u}{\mu k}\right)}{e} \tag{6.61}$$

$$e \cdot \cos(\theta - \theta') + 1 = \frac{\ell^2}{\mu k} u$$

Only 3 of 4 constants appear in the orbit equation

$$u = \frac{1}{r} = \frac{\mu k}{\ell^2}\left(1 + e \cdot \cos(\theta - \theta')\right) \tag{6.62}$$

$\theta' =$ turning point of orbit

Constants: E, ℓ, θ', θ_o [$\theta_o =$ initial position]

$$r = \frac{a(1 - e^2)}{[1 + e \cdot \cos(\theta - \theta')]} \tag{6.63}$$

where a is the semimajor axis

$$a = \frac{1}{2}(r_1 + r_2) \tag{6.64}$$

$$= \frac{-k}{2E}$$

Equation for a conic with one focus at the origin:
$e =$ "eccentricity" and ellipse axis: $a(1-e)$ and $a(1+e)$

$$\begin{aligned} e =& \sqrt{1 + \frac{2E\ell^2}{\mu k^2}} \\ =& \sqrt{1 - \frac{\ell^2}{\mu k a}} \end{aligned} \tag{6.65}$$

Aside: In the Bohr model for the atom:

$$\begin{aligned} E = T + V =& \frac{1}{2}\frac{\ell^2}{\mu r^2} - \left(\frac{e^2}{4\pi\epsilon_o}\right)\frac{1}{r} \\ =& \frac{1}{2}\left(\frac{\ell^2}{\mu}\right)u^2 - \left(\frac{e^2}{4\pi\epsilon_o}\right)u \end{aligned} \tag{6.66}$$

$$\frac{dE}{du} = \frac{\ell^2}{\mu}u - \left(\frac{e^2}{4\pi\epsilon_o}\right) = 0 \tag{6.67}$$

leads to:

$$U^* = \frac{\mu}{\ell^2}\left(\frac{e^2}{4\pi\epsilon_o}\right) = \frac{1}{r^*} \tag{6.68}$$

$$r^* = \frac{\ell^2}{\mu}\left(\frac{4\pi\epsilon_o}{e^2}\right) \tag{6.69}$$

$$E^* = -\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_o r^*}\right) \tag{6.70}$$

If ℓ is chosen to be quantized: $\ell = n\hbar$, $n = 1{,}2\ldots$

Note:

$$a_o \equiv \frac{4\pi\epsilon_o \cdot \hbar^2}{e^2 m_e}$$

The Bohr atom radii and energy states:

$$r_n = \frac{n^2\hbar^2}{\mu}\left(\frac{4\pi\epsilon_o}{e^2}\right) \tag{6.71}$$

$$E_n = -\frac{1}{2}\cdot\frac{e^2}{4\pi\epsilon_o}\cdot\frac{1}{r_n} \tag{6.72}$$

The equation for the motion it time for the Kepler problem:

$$t = \sqrt{\frac{\mu}{2}}\int_{r_o}^{r}\frac{dr}{\sqrt{E + \frac{k}{r} - \frac{\ell^2}{2\mu r^2}}} \tag{6.73}$$

$$= \frac{\ell^3}{\mu k^2}\int_{\theta_o}^{\theta}\frac{d\theta}{[1 + e\cdot\cos(\theta - \theta')]^2} \tag{6.74}$$

$$= \frac{\ell^3}{2\mu k^2}\int_0^{\tan\left(\frac{\theta}{2}\right)}(1 + x^2)dx \quad \text{for } e = 1 \tag{6.75}$$

or:

$$t = \frac{\ell^3}{2\mu k^2}\left(\tan\frac{\theta}{2} + \frac{1}{3}\tan^3\frac{\theta}{2}\right) \tag{6.76}$$

Parabolic motion. Hard to invert!

Introduce auxiliary variable Ψ (the eccentric anomaly)

$$r = a(1 - e\cos\Psi)$$

$$\begin{aligned} t(\Psi) =& \sqrt{\frac{\mu a^3}{k}}\int_0^{\Psi}(1 - e\cos\Psi)d\Psi \\ =& \sqrt{\frac{\mu}{k}}a^{\frac{3}{2}}(\Psi - e\sin\Psi) \end{aligned} \tag{6.77}$$

$$\begin{aligned} \tau =& t(2\pi) \\ =& 2\pi\sqrt{\frac{\mu}{k}}a^{\frac{3}{2}} \quad \text{(period)} \end{aligned} \tag{6.78}$$

$$\tag{6.79}$$

Note: Kepler's 3^{rd} law, $K = +G(m_1 \cdot m_2)$, for all planets $m_2 =$ mass of the sun. (6.80)

$$\tau = \frac{2\pi a^{\frac{3}{2}}}{\sqrt{G(m_1 \cdot m_2)}} \sim C \cdot a^{\frac{3}{2}}$$

$$\begin{aligned} \omega =& \frac{2\pi}{\tau} \quad \text{(Revolution frequency)} \\ =& \sqrt{\frac{k}{\mu a^3}} \\ =& \sqrt{\frac{k}{\mu}}\left(\frac{1}{a^{\frac{3}{2}}}\right) \end{aligned} \tag{6.81}$$

6.9 The Laplace-Runge-Lenz Vector

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - \mu k\frac{\mathbf{r}}{r} \tag{6.82}$$

$$V = \frac{-k}{r} \tag{6.83}$$

$$\tag{6.84}$$

$$\begin{aligned} \mathbf{f}(r) =& \frac{-k}{r^2}\left(\frac{\mathbf{r}}{r}\right) \\ =& f(r)\frac{\mathbf{r}}{r} \end{aligned} \tag{6.85}$$

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = -mf(r)r^2\frac{d}{dt}\left(\frac{\mathbf{r}}{r}\right) \tag{6.86}$$

for:

$$\begin{aligned} f(r) =& \frac{-k}{r^2} \\ =& \frac{d}{dt}\left(\frac{\mu k \mathbf{r}}{r}\right) \end{aligned} \tag{6.87}$$

Note: $\mathbf{A} \cdot \mathbf{L} = 0$ and $\mathbf{A} \cdot \mathbf{p} = 0$, $\mathbf{A}$? in plane of orbit.

Chapter 7

Scattering

7.1 Introduction

I = intensity (flux density) of incident particles

$$\begin{aligned} \sigma(\Omega)d\Omega &= \text{scattering cross section (differential scattering cross section)} \\ &= \text{number of particles scattered into solid angle } d\Omega \\ &\quad \text{(about } \Omega\text{) per unit time} \end{aligned}$$

Incident intensity (Symmetry about axis of incident beam)

$$d\Omega \equiv 2\pi \sin\theta d\theta$$

$$\Theta = \text{ scattering angle}$$

$$\begin{aligned} s &= \text{impact parameter} \\ &= \frac{\ell}{mv_o} \\ &= \frac{\ell}{\sqrt{2mE}} \\ &= S(\theta, E) \end{aligned}$$

ℓ = angular momentum and E = energy

r_m = distance of periapsis

$$\Theta = \pi - 2\Psi \tag{7.1}$$

$$\sin\Theta\sigma(\Theta)|d\Theta| = s|ds| \tag{7.2}$$

$$\sigma(\Theta) = \frac{s}{\sin\Theta}\left|\frac{ds}{d\Theta}\right| \tag{7.3}$$

(Assume one-to-one mapping $s \leftrightarrow \Theta$)

Recall:

$$\Theta = \int_{r_o}^{r} \frac{dr}{r^2\sqrt{\frac{2\mu E}{\ell^2} - \frac{2\mu V}{\ell^2} - \frac{1}{r^2}}} + \underbrace{\Theta_o}_{\pi} \tag{7.4}$$

$\theta = n - \Psi$ when $r - r_m$ (for $\theta_o = \pi$ and $r_o = \infty$)

$$\Psi = \int_{r_m}^{\infty} \frac{dr}{r^2\sqrt{\frac{2\mu E}{\ell^2} - \frac{2\mu V}{\ell^2} - \frac{1}{r^2}}} \tag{7.5}$$

$$\Psi = \int_{r_m}^{\infty} \frac{dr}{r^2\sqrt{\frac{2\mu}{\ell^2}[E - V(r)] - \frac{1}{r^2}}} = \Psi(E, \ell) \tag{7.6}$$

Note: $\dot{\theta} = \frac{\ell}{\mu r^2}$ = constant, hence it cannot change sign (is monotonic in time)

Want Ψ in terms of S and E.

$$E = \frac{1}{2}\mu V_\infty^2 \tag{7.7}$$

$$|\ell| = \ell = |\mathbf{r} \times \mathbf{p}| = \text{ constant}$$

$$\mathbf{r} \times \mathbf{p} = \begin{matrix} \hat{x} & \hat{y} & \hat{z} \\ \infty & s & 0 \\ \mu V_\infty & 0 & 0 \end{matrix}$$

$$= \mu V_\infty s \hat{z}$$

$$\ell = \mu V_\infty s \qquad E = \frac{1}{2}\mu V_\infty^2 \qquad \mu V_\infty = \sqrt{2\mu E}$$

$$\ell = s \cdot \sqrt{2\mu E} \tag{7.8}$$

$$\begin{aligned} \Theta(s) &= \pi - 2\Psi \\ &= \pi - 2\int_{r_m}^{\infty} \frac{s\,dr}{r\sqrt{r^2\left(1 - \frac{V(r)}{E}\right) - s^2}} \\ &= \pi - 2\int_0^{u_m} \frac{s\,du}{\sqrt{1 - \frac{V\left(\frac{1}{u}\right)}{E} - s^2u^2}} \end{aligned} \tag{7.9}$$

$$\frac{2\mu}{\ell^2} = \frac{2\mu}{s^2 \cdot 2\mu E} = \frac{1}{s^2 E}$$

With $\ell = S\sqrt{2\mu E}$ and $\Theta(S) = \pi - 2\Psi$

$$\Theta(s) = \pi - 2\int_{r_m}^{\infty} \frac{s \cdot dr}{r\sqrt{r^2\left(1 - \frac{V(r)}{E}\right) - s^2}} \tag{7.10}$$

$$u = \frac{1}{r} \qquad r = \frac{1}{u} \qquad dr = -\frac{du}{u^2} \tag{7.11}$$

$$u_m = \frac{1}{r_m} \qquad u_\infty = 0 \tag{7.12}$$

$$\Theta(s) = \pi - 2\int_{0}^{u_m} \frac{s \cdot du}{\sqrt{1 - \frac{V(\frac{1}{u})}{E} - s^2u^2}} \tag{7.13}$$

Scattering in a Coulomb field

$$V = \frac{ZZ'}{r} \text{ (atomic units)}$$

For $E > 0$,

$$\begin{aligned} e &= \sqrt{1 + \frac{2El^2}{\mu(ZZ')^2}} \\ &= \sqrt{1 + \left(\frac{2Es}{ZZ'}\right)^2} \end{aligned} \tag{7.14}$$

$$\frac{1}{r} = \mu\left(\frac{ZZ'}{\ell^2}\right)[\epsilon\cos(\theta - \theta') - 1], \text{ let } \theta' = \pi$$

$$\lim_{r\to\infty}\frac{1}{r} = 0, \text{ hence } \quad \epsilon\cos\overbrace{(\theta - \pi)}^{-\Psi} - 1 = 0$$

$$\begin{aligned} \cos(-\Psi) = \cos\Psi = \frac{1}{\epsilon} &= \cos\left[\frac{\pi}{2} - \frac{\Theta}{2}\right] \\ &= \cos\left[\frac{\Theta}{2} - \frac{\pi}{2}\right] \\ &= \sin\frac{\Theta}{2} = \frac{1}{\epsilon} \end{aligned} \tag{7.15}$$

Solving for:

$$\epsilon^2 = \cot^2\frac{\Theta}{2} + 1 \pm \cos^2\frac{\Theta}{2} \tag{7.16}$$

since:

$$\frac{1}{\sin^2 x} = \frac{\cos^2 x + \sin^2 x}{\sin^2 x} = \cot^2 x + 1$$

$$\cot\frac{\Theta}{2} = \frac{2Es}{ZZ'} \tag{7.17}$$

this gives:

$$S = \frac{ZZ'}{2E}\cot\frac{\Theta}{2} \tag{7.18}$$

recall:

$$\begin{aligned}\sigma(\Theta) =& \frac{S}{\sin\Theta}\frac{|ds|}{|d\Theta|} \\ =& \frac{1}{4}\left(\frac{ZZ'}{2E}\right)^2 \csc^4\frac{\Theta}{2}\end{aligned} \tag{7.19}$$

7.2 Rutherford Scattering

7.2.1 Rutherford Scattering Cross Section

(Rutherford experiment...)

Total scattering cross section:

$$\begin{aligned}\sigma_T =& \int d\Omega\sigma(\Omega) \\ =& 2\pi\int_0^\pi d\Theta\sin\Theta\sigma(\Theta)\end{aligned} \tag{7.20}$$

Really, Θ not a single-values function of s

$$\sigma(\Theta) = \sum_i \frac{s_i}{\sin\Theta}\left|\frac{ds}{d\Theta}\right| \tag{7.21}$$

Rainbow scattering (E of particle exceeds V_m, goes through)

Glory scattering (orbiting/spinaling occurs...)

7.2.2 Rutherford Scattering in the Laboratory Frame

$$\tan\theta_1 = \frac{m_2\sin\Theta}{m_1 + m_2\cos(\Theta)} \tag{7.22}$$

$$\underbrace{\theta_2 = \frac{1}{2}(\pi - \Theta)}_{\Theta=\pi-2\theta_2} \tag{7.23}$$

Scattering Particle:

$$\sigma_2(\Theta_2) = \left(\frac{ZZ'}{2E}\right)^2 \cdot \sec^3\theta_2 \tag{7.24}$$

$$\sigma_1(\theta_1) = \text{ difficult } \ldots \tag{7.25}$$

Case I:

$$m_2 >> m_1 \qquad \Theta \approx \theta_1 \qquad \mu \sim m_1$$

$$\sigma_1(\theta_1) = \frac{1}{u}\left(\frac{ZZ'}{2E_1}\right)^2 \csc^4\left(\frac{\theta_1}{2}\right) \qquad \text{(same result)} \tag{7.26}$$

Case II:

$$m_1 = m_2 = m \qquad \mu = \frac{m}{2} \qquad \Theta = 2\theta_1$$

"x" in fig. $\theta_1 + \theta_2 = \frac{\pi}{2}$

$$\sigma_1(\theta_1) = \left(\frac{ZZ'}{E_1}\right)^2 \frac{\cos\theta_1}{\sin^4\theta_1} \tag{7.27}$$

For identical particles, cannot tell which is "scattered", so:

$$\sigma_1(\theta) = \left(\frac{ZZ'}{E_1}\right)^2 \left(\frac{1}{\sin^4\theta} + \frac{1}{\cos^4\theta}\right)\cos\theta \tag{7.28}$$
$$= \left(\frac{ZZ'}{E_1}\right)^2 \left[\csc^4\theta + \sec^4\theta\right]\cos\theta$$

7.3 Examples

$$E \geq V' \geq V$$

$$E_4 = \text{ circular} \tag{7.29}$$
$$E_3 = \text{ elliptic} \tag{7.30}$$
$$E_2 = \text{ parabolic} \tag{7.31}$$
$$E_1 = \text{ hyperbolic} \tag{7.32}$$

r_1, r_2 = apsidal distances (turning points) for bounded motion.

r_o is solution of:

$$\left.\frac{dV'}{dr}\right|_{r_o} = 0$$

(Circular orbit)

$$r = \frac{a(1-e^2)}{1 + e\cdot\cos(\theta - \theta')}$$

$$e = \sqrt{1 + \frac{2E\ell^2}{\mu K^2}}$$

Chapter 8

Collisions

Collisions...

$$\mathbf{P}'_1 = \mu \mathbf{V}_o + \mu \frac{\mathbf{P}}{m_2} \quad (8.1)$$

$$\mathbf{P}'_2 = -\mu \mathbf{V}_o + \mu \frac{\mathbf{P}}{m_1} \quad (8.2)$$

$$\mathbf{AB} = \mathbf{P} \qquad \mathbf{OC} = \mu \mathbf{V}_o$$

$$\frac{AO}{OB} = \frac{m_1}{m_2} \qquad \mathbf{AO} = \mu \frac{\mathbf{P}}{m_2}$$

$$\mathbf{OB} = \mu \frac{\mathbf{P}}{m_1}$$

If m_2 is initially at rest ($|OB| = \mu \nu_o$)

$$\tan \theta_1 = \frac{m_2 \sin x}{m_1 + m_2 \cos x} \qquad \theta_2 = \frac{1}{2}(\pi - x) \quad (8.3)$$

In center of mass reference frame (i.e. moving with the center of mass) - total $\mathbf{P} = 0$ for this frame...

$$E_i = \left(E_{1i} + \frac{P_o^2}{2m_1}\right) + \left(E_{2i} + \frac{P_o^2}{2m_2}\right) \quad (8.4)$$

$$E_i = \text{ internal energy}$$

$$\mathbf{P}_1 = m_1 \mathbf{v}_1 \quad (8.5)$$

$$T = \frac{\mathbf{P}_1^2}{2m_1} = \frac{\mathbf{P}_o^2}{2m_1} \quad (8.6)$$

$$|\mathbf{P}_1| = |\mathbf{P}_2| = P_o \quad (8.7)$$

$$\mathbf{P}_2 = m_2 \mathbf{v}_2 = -\mathbf{P}_1 \quad (8.8)$$

$$T = \frac{\mathbf{P}_2^2}{2m_2} = \frac{\mathbf{P}_o^2}{2m_2} \tag{8.9}$$

$$\epsilon = E_i - (E_{1i} + E_{2i}) \tag{8.10}$$
$$= \text{“disintegration energy”} > 0 \tag{8.11}$$
$$= \frac{1}{2} P_o^2 \left(\frac{1}{m_1} + \frac{1}{m_2} \right) = \frac{P_o^2}{2\mu}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

In laboratory center of mass reference frame, $\mathbf{V}$ = velocity of primary particle prior to disintegration.

$$\mathbf{V} = \mathbf{v} - \mathbf{v}_o \tag{8.12}$$
$$\mathbf{v} = \mathbf{V} + \mathbf{v}_o \tag{8.13}$$
$$\mathbf{v}_o = \mathbf{v} - \mathbf{V} \tag{8.14}$$

$\mathbf{v}$ = velocity of one of the particles (in L frame) after disintegration
$\mathbf{v}_o$ = velocity of one of the particles (in C frame) after disintegration

8.1 Elastic Collisions

No change in the internal energy of colliding particles.

In center of mass reference frame ($\mathbf{P} = 0$), let:

$$P_o \hat{n}_o = \mu \mathbf{v}_o \tag{8.15}$$
$$\mathbf{v}_o \equiv \frac{P_o}{\mu} \hat{n}_o \tag{8.16}$$

$$\mathbf{P}'_{o1} = m_1 \mathbf{v}'_{o1} \tag{8.17}$$
$$= -\mathbf{P}'_{o2} \tag{8.18}$$
$$= P_o \hat{n}_o \tag{8.19}$$

$$|\mathbf{P}'_{o1}| = |\mathbf{P}'_{o2}| = P_o \tag{8.20}$$

$$m_1 \mathbf{v}'_{o1} = -m_2 \mathbf{v}'_{o2} \tag{8.21}$$

$$\mathbf{P}'_{o2} = m_2 \mathbf{v}'_{o2} = -\mathbf{P}'_{o1} = -P_o \hat{n}_o$$

Primes $\rightarrow$ after collision

$$m_1 \mathbf{v}'_{o1} = P_o \hat{n}_2 \qquad m_1 v'_{o1} = P_o \qquad v'_{o1} = \frac{P_o}{m_1} \tag{8.22}$$

$$\mathbf{v}'_{o1} = \frac{m_2 \mathbf{v}_o}{m_1 + m_2} = \frac{P_o}{m_1} \hat{n}_o \tag{8.23}$$

$$\mathbf{v}'_{o2} = \frac{-m_1 \mathbf{v}_o}{m_1 + m_2} = \frac{-P_o}{m_2} \hat{n}_o \tag{8.24}$$

In "L" reference frame:

$$\mathbf{P} = \mathbf{P}_1 + \mathbf{P}_2 \qquad \mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2 \tag{8.25}$$

$$\mathbf{v}'_1 = \mathbf{v}'_{10} + \boldsymbol{\nabla} \tag{8.26}$$

$$\mathbf{v}'_2 = \mathbf{v}'_{20} + \boldsymbol{\nabla} \tag{8.27}$$

$$\boldsymbol{\nabla} = \frac{\mathbf{P}}{m} = \frac{m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2}{m_1 + m_2} \tag{8.28}$$

$$\mathbf{P}'_1 = P_o \hat{n}_o + (\mathbf{P}_1 + \mathbf{P}_2) \frac{m_1}{m_1 + m_2} = \mu \left[\mathbf{v}_o + \frac{\mathbf{P}}{m_2} \right] \tag{8.29}$$

$$\mathbf{P}'_2 = - P_o \hat{n}_o + (\mathbf{P}_1 + \mathbf{P}_2) \frac{m_2}{m_1 + m_2} = \mu \left[-\mathbf{v}_o + \frac{\mathbf{P}}{m_1} \right] \tag{8.30}$$

If m_2 is initially at rest ($\mathbf{P}_2 = 0$) then:

$$\tan\theta_1 = \frac{m_2 \sin x}{m_1 + m_2 \cos x} \qquad \theta_2 = \frac{1}{2}(\pi - x) \tag{8.31}$$

$$\nu'_1 = \frac{|\mathbf{P}'_1|}{m_1} = \frac{\sqrt{(m_1^2 + m_2^2 + 2 m_1 m_2 \cos x)}}{m_1 + m_2} \nu \tag{8.32}$$

$$\nu'_2 = \frac{|\mathbf{P}'_2|}{m_2} = \frac{2 m_1 \nu}{m_1 + m_2} \sin \frac{1}{2} x \tag{8.33}$$

- For head on collisions, $x = \pi$ and $\mathbf{P}_1$ and $\mathbf{P}_2$ are in the same ($m_1 > m_2$) or opposite ($m_1 < m_2$) directions.
- In this case (head-on collision):

$$\mathbf{v}'_1 = \frac{m_1 - m_2}{m_1 + m_2} \mathbf{v} \qquad \mathbf{v}'_2 = \frac{2 m_1}{m_1 + m_2} \mathbf{v} \tag{8.34}$$

$$E_1 = \frac{1}{2} m_1 v^2 \qquad E'_{2max} = \frac{4 m_1 m_2}{(m_1 + m_2)^2} E_1 \tag{8.35}$$

For head-on collision, if $m_1 = m_2$, then m_1 stops and transfers all of it's energy to m_2.

- If $m_1 < m_2$ then m_1 can bounce off m_2 and have velocity in any direction.

- If $m_1 >_2$, it cannot "bounce back" (become reflected) and there is an angle θ_{max} for which the deflected angle θ_1 must lie within $-\theta_{max} \leq \theta_1 \leq \theta_{max}$

$$\sin\theta_{max} = \frac{m_2}{m_1} \tag{8.36}$$

If $m_1 = m_2$, then $\theta_1 + \theta_2 = \frac{\pi}{2}$:

$$\theta_1 = \frac{1}{2}x \qquad \theta_2 = \frac{1}{2}(\pi - x) \tag{8.37}$$

$$\nu_1' = \nu\cos\frac{1}{2}x \qquad \nu_2' = \nu\sin\frac{1}{2}x \tag{8.38}$$

and after collision, particles move at right angles to one-another.

Chapter 9

Oscillations

9.1 Euler Angles of Rotation

Euler's Theorem: The general displacement of a rigid body with one point fixed is a rotation about some axis.

Chasles' Theorem: The most general displacement of a rigid body is a translation plus a rotation.

$$u(x) = \frac{1}{2}kx^2 \qquad P(x) \sim e^{-\beta u(x)}$$

$$x(t) = A\sin(\omega t + \phi) \tag{9.1}$$

$$p(t)dt = \frac{dx}{2\pi\sqrt{A^2 - x^2}} \qquad \text{(Classical, microcanonical)} \tag{9.2}$$

$$|\Psi_o|^2 \sim e^{-\alpha x^2} \qquad \alpha = \sqrt{\frac{ku}{\hbar^2}}$$

$$\int_o^{\frac{2\pi}{\omega}} p(t)dt = \frac{1}{2\pi}\sin^{-1}\left(\frac{x}{A}\right) \tag{9.3}$$

9.2 Oscillations

Consider a conservative system with generalized coordinates whose transformation are independent of time (i.e. constraints are independent of time and $T = T_2-$quadratic).

At equilibrium:

$$Q_i = -\left(\frac{\partial V}{\partial q_i}\right)_o = 0 \tag{9.4}$$

$$V(\mathbf{q}) = V^{(o)}(\mathbf{q}_o) + \delta\mathbf{q}^T \cdot \mathbf{V}^{(1)} + \frac{1}{2}\delta\mathbf{q}^T \cdot \mathbf{V}^{(2)} \cdot \delta\mathbf{q} + \dots$$

$$\left(-\mathbf{V}_o^{(1)}\right)_i = \left.\frac{\partial V}{\partial q_i}\right|_o \qquad \left(\mathbf{V}_o^{(2)}\right)_{ij} = \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_o$$

So, for small displacements $\delta\mathbf{q}$ about the equilibrium $\mathbf{q}_o$, we have:

$$V(\mathbf{q}) - V(\mathbf{q}_o) = \Delta V q = \frac{1}{2}\delta\mathbf{q}^T \cdot \mathbf{V}^{(2)} \cdot \delta\mathbf{q} \tag{9.5}$$

$$T = \frac{1}{2}\sum_{ij} T_{ij}^{(2)} \dot{q}_i \dot{q}_j \tag{9.6}$$

where:

$$T_{ij}^{(2)} \equiv \sum_k m_k \frac{\partial \mathbf{r}_i}{\partial q_i} \cdot \frac{\partial \mathbf{r}_j}{\partial q_j} = m_{ij}(q_1 \dots q_N) \tag{9.7}$$

$$(q \dot{-} q_o) = \delta\dot{q} = \dot{q}$$

$$\begin{aligned} T =& \frac{1}{2}\dot{\mathbf{q}}^T \cdot \mathbf{T}^{(2)} \cdot \dot{\mathbf{q}} && (9.8) \\ =& \frac{1}{2}\delta\dot{\mathbf{q}}^T \cdot \mathbf{T}^{(2)} \cdot \delta\dot{\mathbf{q}} \\ \approx& \frac{1}{2}\delta\dot{\mathbf{q}}^T \cdot \mathbf{T}_o^{(2)} \cdot \delta\dot{\mathbf{q}} && (9.9) \end{aligned}$$

where:

$$\mathbf{T}_o^{(2)} = \mathbf{T}^{(2)}(\mathbf{q}_o)$$

Note:

$$\mathbf{T}^{(2)} = \mathbf{T}^{(2)}(q)$$

$$\begin{aligned} T_{ij}^{(2)}(\mathbf{q}) =& T_{ij}^{(2)}(\mathbf{q}_o) + \delta\mathbf{q}^T \cdot \left(\frac{\partial T_{ij}^{(2)}}{\partial \mathbf{q}}\right) + \frac{1}{2}\delta\mathbf{q}^T \cdot \left(\frac{\partial^2 T_{ij}^{(2)}}{\partial \mathbf{q}\partial \mathbf{q}}\right)\delta\mathbf{q} + \dots \\ \sim& \underbrace{T_{ij}^{(2)}(\mathbf{q_o})}_{\mathbf{T}_o^{(2)}} \end{aligned}$$

for small $\delta\mathbf{q} \equiv \mathbf{q} - \mathbf{q}_o$

So,

$$\begin{aligned} \Delta V =& V(\mathbf{q}) - V(\mathbf{q}_o) && (9.10) \\ =& \frac{1}{2}\delta\mathbf{q}^T \cdot \mathbf{V}_o^{(2)} \cdot \delta\mathbf{q} \end{aligned}$$

Note: the zero of the potential is arbitrary

$$T = \frac{1}{2}\delta\dot{\mathbf{q}}^T \cdot \mathbf{T}_o^{(2)} \cdot \delta\dot{\mathbf{q}} \tag{9.11}$$

$$\begin{aligned} L =& T - \Delta V && (9.12) \\ =& \frac{1}{2}\left[\delta\dot{\mathbf{q}}^T \cdot \mathbf{T}_o^{(2)}\delta\dot{\mathbf{q}} + \delta\dot{\mathbf{q}}^T \cdot \mathbf{V}_o^{(2)} \cdot \delta\mathbf{q}\right] \end{aligned}$$

$$\frac{dL}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial L}{\partial \mathbf{q}} = \mathbf{T}_o^{(2)} \cdot \delta\ddot{\mathbf{q}} + \mathbf{V}_o^{(2)}\delta\mathbf{q} = 0 \tag{9.13}$$

Note: $\frac{d}{dt}\left(\mathbf{T}_o^{(2)}\right) = \mathbf{0}$ since the equation of transformation are independent of time, and $\mathbf{T}_o^{(2)} = \mathbf{T}^{(2)}(\mathbf{q}_o)$

Note: in Cartesian coordinates,

$$(\mathbf{q}) = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \\ \vdots \\ x_{\frac{N}{3}} \\ y_{\frac{N}{3}} \\ z_{\frac{N}{3}} \end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix}$$

$$\left(\mathbf{T}_o^{(2)}\right)_{ij} = m_{\alpha_i} \cdot \delta_{ij} \quad \text{where } \alpha_i = moD(i,3)$$

e.g.

$$\begin{pmatrix} m_1 & & & & & & \\ & m_1 & & & & & \\ & & m_1 & & & & \\ & & & m_2 & & & \\ & & & & m_2 & & \\ & & & & & m_2 & \\ & & & & & & \ddots \end{pmatrix}$$

and in mass-weighted Cartesian coordinates:

$$x_i' = \frac{x_i}{\sqrt{M_i}} \qquad \left(\mathbf{T}_o^{(2)}\right)_{ij} = \delta_{ij}$$

let:

$$\delta q_k = C - a_k \cdot \cos(\omega t - \phi) \qquad \delta\ddot{q}_k = -\omega^2 \delta q_k$$

Note: the δq_k's are functions of time, and the a_k's are linear algebraic coefficients to be solved for.

$$\left(\mathbf{V}_o^{(2)} - \omega^2 \mathbf{T}_o^{(2)}\right)\delta\mathbf{q} = 0 \tag{9.14}$$

$$\mathbf{V}_o^{(2)}\mathbf{a}_k = \omega_k^2 \mathbf{T}_o^{(2)}\mathbf{a}_k \tag{9.15}$$

$$\mathbf{V}_o^{(2)}\mathbf{A} = \mathbf{T}_o^{(2)}\mathbf{A} \cdot \boldsymbol{\omega}^2 \tag{9.16}$$

(A generalized eigenvector problem that have non-trivial solutions when ω^2 is a root of the secular equation. Note that $\mathbf{V}$ and $\mathbf{T}$ are real symmetric.)

We learned previously that the solution of a generalized eigenvector problem involving Hermitian matrices results in a set of eigenvectors that are bi-orthogonal with real eigenvalues. Note:

$$\mathbf{V}_o^{(2)}\mathbf{A} = \mathbf{T}_o^{(2)} \cdot \mathbf{A} \cdot \boldsymbol{\omega}^2 \tag{9.17}$$

Dropping superscrips and subscripts.

$$(\mathbf{T}^{-\frac{1}{2}} \cdot \mathbf{V} \cdot \mathbf{T}^{-\frac{1}{2}})\mathbf{T}^{\frac{1}{2}}\mathbf{A} = \mathbf{T}^{-\frac{1}{2}}\mathbf{T}\mathbf{T}^{-\frac{1}{2}}\mathbf{T} \cdot \mathbf{A} \cdot \boldsymbol{\omega}^2 \tag{9.18}$$

Regular eigenvector problem:

$$\mathbf{V}'\mathbf{A} = \mathbf{A}'\boldsymbol{\omega}^2$$

$$\boldsymbol{\omega}^2 = \mathbf{A}'^T \cdot \mathbf{V}' \cdot \mathbf{A}'$$

if $\mathbf{A}'$ is normalized such that $\mathbf{A}'^T \cdot \mathbf{A} = \mathbf{1}$ in which case:

$$\mathbf{A}'^T = \mathbf{A}^{-1} \qquad (\mathbf{A} \text{ is orthogonal})$$

or

$$\omega_k^2 = \frac{\mathbf{a}_k'^T \cdot \mathbf{V}'\mathbf{a}_k}{\mathbf{a}_k'^T \cdot \mathbf{a}_k}$$

if all $\omega_k^2 > 0$, all $\omega_k > 0 \quad \rightarrow \quad$ minimum.
if one $\omega_k^2 < 0$, that ω_k is imaginary $\rightarrow$ "transition state" (1^{st} order saddle point)
if n of the $\omega_k^2 < 0$, those ω_k are imaginary, "n^{th} order saddle point"

$$\mathbf{V}_o^{(2)}\mathbf{A} = \mathbf{T}_o^{(2)}\mathbf{A}\boldsymbol{\omega}^2 \tag{9.19}$$

$$\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2 \ldots \mathbf{a}_N)\mathbf{a}_k$$

Choose normalization such that:

$$\mathbf{A}^T\mathbf{V}_o^{(2)}\mathbf{A} = \boldsymbol{\omega}^2 \qquad \text{(diagonal)} \qquad \mathbf{A}^T\mathbf{T}_o^{(2)}\mathbf{A} = \mathbf{1}$$

9.3 General Solution of Harmonic Oscillator Equation

9.3.1 1-Dimension

$$\frac{d^2}{dt^2}q(t) = -\omega^2 q(t) \tag{9.20}$$

$$
\begin{aligned}
q(t) =& C_1 e^{i\omega t} + C_2 e^{-i\omega t} && \left(C_3 \frac{\left[e^{i\omega t} - e^{-i\omega t}\right]}{2i} + C_4 \ldots \right) \\
=& C_3 \sin(\omega t) + C_4 \cos(\omega t) \\
=& C_5 \sin[\omega t + C_6] \\
=& C_7 \cos[\omega t + C_7] \\
& \vdots
\end{aligned}
\tag{9.21}
$$

e.g.

$$
q(0) = q_o \qquad \dot{q}(0) = 0 \tag{9.22}
$$

$$
C_4 = q_o \qquad \omega C_3 = 0 \qquad C_3 = 0
$$

$$
q(t) = q_o \cos \omega t
$$

e.g.

$$
q(t_o) = 0 \qquad \dot{q}(t_o) = v_o
$$

$$
C_\beta = -\omega t_o \qquad \omega C_5 = v_o \qquad C_5 = \frac{v_o}{\omega}
$$

$$
q(t) = \frac{v_o}{\omega} \sin[\omega(t - t_o)]
$$

9.3.2 Many-Dimension

Normal coordinates

$$
\delta q_i(t) = \sum_k C_k a_{ik} \cos[\omega t + \phi_k] \qquad \text{or equivalent}
$$

let:

$$
\underbrace{\delta \mathbf{q}' = \mathbf{A}^T \cdot \delta \mathbf{q}}_{\delta q'_k = (\mathbf{a}_k^T \cdot \delta \mathbf{q}) \mathbf{a}_k}
$$

(Projection in orthogonal coordinates)

or

$$
\delta \mathbf{q} = \mathbf{A} \quad \delta \mathbf{q}'
$$

$$\begin{aligned} V =& \frac{1}{2}\delta\mathbf{q}^T \cdot \mathbf{V}_o^{(2)} \cdot \delta\mathbf{q} \\ =& \frac{1}{2}\delta\mathbf{q}'^T \cdot \underbrace{\mathbf{A}^T \cdot \mathbf{V}_o^{(2)}\mathbf{A}}_{\boldsymbol{\omega}^2} \delta\mathbf{q}' \\ =& \frac{1}{2}\delta\mathbf{q}'^T \cdot \boldsymbol{\omega}^2 \cdot \delta\mathbf{q}' \\ =& \frac{1}{2}\sum_k \omega_k^2 \cdot \delta q_k'^{\,2} \end{aligned} \tag{9.23}$$

$$\begin{aligned} T =& \frac{1}{2}\delta\mathbf{q}^T \cdot \mathbf{T}_o^{(2)} \cdot \delta\mathbf{q} \\ =& \frac{1}{2}\delta\mathbf{q}'^T \cdot \underbrace{\mathbf{A}^T \cdot \mathbf{T}_o^{(2)}\mathbf{A}}_{?} \cdot \delta\mathbf{q}' \\ =& \frac{1}{2}\delta\mathbf{q}'^T \cdot \delta\mathbf{q}' \\ =& \frac{1}{2}\sum_k \delta\mathbf{q}_k'^{\,2} \end{aligned} \tag{9.24}$$

9.4 Forced Vibrations

$$Q_i' = \sum_i A_{ji} Q_j \qquad (\,\mathbf{Q}' = \mathbf{A}^T \cdot \mathbf{Q}, \mathbf{Q} = \mathbf{A} \cdot \mathbf{Q}')$$

$$\delta\ddot{q}_i' + \omega_i^2 \delta q_i' = Q_i'$$

Suppose $Q_i' = Q_{io}' \cos(\omega t + \delta_i)$ (e.g. the oscillating electromagnetic field of a monochromatic light source on a polyatomic molecule, $\delta q_i'$ are the molecular normal "Raman" vibrational modes)

Note:

$$\ddot{Q}_i' = -\omega^2 Q_{io}' \cos(\omega t + \delta_i) = -\omega^2 Q_i'$$

let $\qquad \delta q_i' = \dfrac{Q_i'}{\omega_i^2 - \omega^2} \qquad$ then $\qquad \delta\ddot{q}_i' = -\,\omega^2 \delta q_i'$

$$\begin{aligned} \delta\ddot{q}_i' + \omega_i^2 \delta q_i' =& -\,\omega^2 \delta q_i' + \omega_i^2 \delta q_i' && (9.25) \\ =& (\omega_i^2 - \omega^2)\delta q_i' \\ =& (\omega_i^2 - \omega^2)\frac{Q_i'}{\omega_i^2 - \omega^2} \\ =& Q_i' && (9.26) \end{aligned}$$

Which is a solution of the desired equation. Hence:

$$\begin{aligned}\delta q_i'(t) =& \frac{Q_i'(t)}{\omega_i^2 - \omega^2} \\ =& \frac{Q_{io}' \cos(\omega t + \delta_i)}{\omega_i^2 - \omega^2}\end{aligned} \tag{9.27}$$

$$\begin{aligned}\delta q_i(t) &= \sum_j A_{ij} \delta q_j'(t) \\ &= \sum_j A_{ij} \frac{Q_{jo}' \cos(\omega t + \delta_j)}{\omega_j^2 - \omega^2}\end{aligned} \tag{9.28}$$

9.5 Damped Oscillations

Recall:

$$\begin{aligned}F =& \frac{1}{2} \sum_i \sum_j F_{ij} \delta\dot{q}_i \delta\dot{q}_j \\ =& \frac{1}{2} \delta\dot{\mathbf{q}}^T \cdot \mathbf{F} \cdot \delta\dot{\mathbf{q}} \\ \approx& \frac{1}{2} \delta\dot{\mathbf{q}}^T \cdot \mathbf{F}_o^{(2)} \cdot \delta\dot{\mathbf{q}}\end{aligned} \tag{9.29}$$

"Lagrange's" equations are:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = Q_j = -\frac{\partial F}{\partial q_j} \tag{9.30}$$

or in matrix form.

$$\mathbf{T}_o^{(2)} \delta\ddot{\mathbf{q}} + \mathbf{F}_o^{(2)} \delta\dot{\mathbf{q}} + \mathbf{V}_o^{(2)} \delta\mathbf{q} = 0 \tag{9.31}$$

It is not possible, in general, to find a principle axis transformation that simultaneously diagonalizes three matices in order to decouple the equations.

In some cases it is possible, however. One example is when frictional forces are proportional to both the particles mass and velocity.

More generally, anytime the transformation that diagonolizes $\mathbf{T}_o^{(2)}$ and $\mathbf{V}_o^{(2)}$ also diagonalizes $\mathbf{F}_o^{(2)}$ with eigenvalues F_i, we have:

$$\delta\ddot{q}_k' + F_k \delta\dot{q}_k' + \omega_k^2 \delta q_k' = 0 \tag{9.32}$$

In that case (use of complex exponentials useful)

$$\delta q_k'(t) = C_k e^{-i\omega_k' t} \qquad \text{leads to:}$$

$$\left[{\omega_k'}^2 + i\omega_k' F_k - \omega_i^2\right] \delta q_k'(t) = 0 \tag{9.33}$$

$$\omega'_k = \pm\sqrt{\omega_k^2 - \frac{F_k^2}{4}} - i\frac{F_k}{2} \tag{9.34}$$

$$ax^2 + bx + c$$
$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$a = 1 \qquad b = iF_k \qquad c = -\omega_k^2$$

Which gives:

$$\delta q'_k(t) = C_k e^{\frac{-F_k t}{2}} e^{-i\omega_k t} \tag{9.35}$$

The general solution is harder. . .

Chapter 10

Fourier Transforms

10.1 Fourier Integral Theorem

$f(\mathbf{r})$ piecewise smooth, absolutely integrable, and if:

$$f(\mathbf{r}) = \frac{1}{2}\left[f(\mathbf{r}^+) + f(\mathbf{r}^-)\right] \tag{10.1}$$

at points of discontinuity, then:

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} \widetilde{f}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3k \tag{10.2}$$

where

$$\begin{aligned} \widetilde{f}(\mathbf{k}) =& F_k(f(\mathbf{r})) \\ =& \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} f(\mathbf{r}') e^{-i\mathbf{k}\cdot\mathbf{r}'} d^3r' \end{aligned} \tag{10.3}$$

Note, this implies:

$$\begin{aligned} f(\mathbf{r}) =& \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3k e^{i\mathbf{k}\cdot\mathbf{r}} \int_{-\infty}^{\infty} d^3r' e^{-i\mathbf{k}\mathbf{r}'} f(\mathbf{r}') \\ =& \int_{-\infty}^{\infty} d^3r' f(\mathbf{r}') \underbrace{\frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} d^3k}_{\delta(\mathbf{r}-\mathbf{r}')} \\ =& \int_{-\infty}^{\infty} d^3r' f(\mathbf{r}') \delta(\mathbf{r}-\mathbf{r}') \end{aligned} \tag{10.4}$$

$$\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} d^3k \tag{10.5}$$

This is the "spectral resolution" of the identity.

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3k e^{i\mathbf{k}\cdot(\mathbf{r})} \widetilde{f}(\mathbf{k}) \qquad \widetilde{f}(\mathbf{k}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r e^{-i\mathbf{k}\cdot(\mathbf{r})} f(\mathbf{r})$$

10.2 Theorems of Fourier Transforms

- Derivative Theorem:

$$F_k\{\nabla f(\mathbf{r})\} = -i\mathbf{k}\widetilde{f}(\mathbf{k}) \tag{10.6}$$

- Convolution Theorem:

$$(f * g)(\mathbf{r}) \equiv \int g(\mathbf{r}')f(\mathbf{r}-\mathbf{r}')d^3r' \tag{10.7}$$

$$F_k\{f * g\} = \frac{1}{(2\pi)^{\frac{3}{2}}}\widetilde{f}(\mathbf{k})\widetilde{g}(\mathbf{k}) \tag{10.8}$$

- Translation Theorem:

$$F_k\{\delta(\mathbf{r}-\mathbf{R}_A)\} = \frac{e^{-i\mathbf{k}\cdot\mathbf{R}_A}}{(2\pi)^{\frac{3}{2}}} \tag{10.9}$$

  and hence:

$$F_k\{f(\mathbf{r}-\mathbf{R}_A)\} = \frac{e^{-i\mathbf{k}\cdot\mathbf{R}_A}}{(2\pi)^{\frac{3}{2}}}\widetilde{f}(\mathbf{k}) \tag{10.10}$$

- Parseval's Theorem:

$$\int_{-\infty}^{\infty} f^*(\mathbf{r})g(\mathbf{r})d^3r = \int_{-\infty}^{\infty} \widetilde{f}(\mathbf{k})^*\widetilde{g}(\mathbf{k})d^3k \tag{10.11}$$

Note: there are other conventions for defining things, for example:

$$f(\mathbf{r}) = \int_{-\infty}^{\infty} d^3k e^{-i\mathbf{k}\cdot\mathbf{r}}\widetilde{f}(\mathbf{k}) \tag{10.12}$$

$$f(\mathbf{k}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} d^3\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}}\ddot{f}(\mathbf{r})\ldots \tag{10.13}$$

10.3 Derivative Theorem Proof

$$F_k\{\nabla_{\mathbf{r}} f(\mathbf{r})\} = \frac{1}{(2\pi)^{\frac{3}{2}}}\int_{-\infty}^{\infty} d^3r e^{-i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{r}} f(\mathbf{r}) \tag{10.14}$$

Note:

$$\nabla_{\mathbf{r}}\left(e^{-i\mathbf{k}\cdot\mathbf{r}}f(\mathbf{r})\right) = \left(\nabla_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}}\right)f(\mathbf{r}) + e^{-i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{r}} f(\mathbf{r}) \tag{10.15}$$

hence

$$\int_{-\infty}^{\infty} d^3r e^{-i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{r}} f(\mathbf{r}) = \tag{10.16}$$

$$\underbrace{\int_{-\infty}^{\infty} d^3r \nabla_{\mathbf{r}}\left(e^{-i\mathbf{k}\cdot\mathbf{r}}f(\mathbf{r})\right)} - \int_{-\infty}^{\infty} d^3r\left(\nabla_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}}\right)f(\mathbf{r}) \tag{10.17}$$

recall the generalized divergence theorem

$$\int_V dV \nabla_{\mathbf{r}} \circ \mathbf{f} = \int_S d\boldsymbol{\sigma} \circ \mathbf{f} \tag{10.18}$$

$$\int_{-\infty}^{\infty} d^3r \nabla_{\mathbf{r}} \left(e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) \right) = \int_{S\to\infty} d\boldsymbol{\sigma} \left(e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) \right) = 0 \tag{10.19}$$

if $\left(|e^{-i\mathbf{k}\cdot\mathbf{r}}| = 1\right) f(\mathbf{r}) \to 0$ at any boundarty s.t. $\int_{S\to\infty} d\boldsymbol{\sigma} |f(\mathbf{r})| = 0$ then we have:

$$F_k\{\nabla_{\mathbf{r}} f(\mathbf{r})\} = -\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r \nabla_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) \tag{10.20}$$

$$= + i\mathbf{k} \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r})$$

$$= + i\mathbf{k} \widetilde{f}(\mathbf{k})$$

10.4 Convolution Theorem Proof

$$h(\mathbf{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3k e^{i\mathbf{k}\cdot\mathbf{r}} \underbrace{\widetilde{f}(\mathbf{k})\widetilde{g}(\mathbf{k})}_{\widetilde{h}(\mathbf{k})} \tag{10.21}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3k e^{i\mathbf{k}\cdot\mathbf{r}} g(\mathbf{k}) \cdot \underbrace{\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r' e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}')}_{\widetilde{f}(\mathbf{k})}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r' f(\mathbf{r}') \underbrace{\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3k e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \widetilde{g}(\mathbf{k})}_{g(\mathbf{r}-\mathbf{r}')}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r' f(\mathbf{r}') g(\mathbf{r}-\mathbf{r}')$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} f * g$$

10.5 Parseval's Theorem Proof

$$\int_{-\infty}^{\infty} d^3k \widetilde{f}^*(E) g(\mathbf{k}) = \int_{-\infty}^{\infty} d^3k \left[\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r e^{i\mathbf{k}\cdot\mathbf{r}} \widetilde{f}^*(\mathbf{r}) \right] \widetilde{g}(\mathbf{k}) \tag{10.22}$$

$$= \int_{-\infty}^{\infty} d^3k \cdot \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3r \widetilde{f}^*(\mathbf{r}) \int_{-\infty}^{\infty} d^3r' g(\mathbf{r}') e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

$$= \int_{-\infty}^{\infty} d^3r f(\mathbf{r}) \int_{-\infty}^{\infty} d^3r' g(\mathbf{r}') \underbrace{\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3k e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}_{\delta(\mathbf{r}-\mathbf{r}')}$$

$$= \int_{-\infty}^{\infty} d^3r f(\mathbf{r}) g(\mathbf{r})$$

$$\nabla^2 \phi(\mathbf{r}) = -4\pi\rho(\mathbf{r})$$

$$-k^2 \widetilde{\phi}(\mathbf{k}) = -4\pi\widetilde{\rho}(\mathbf{k}) \qquad \widetilde{\phi}(\mathbf{k}) = 4\pi \frac{\widetilde{\rho}(\mathbf{k})}{k^2}$$

for Gaussian,

$$\widetilde{\phi}(\mathbf{k}) = 4\pi \cdot \frac{e^{\frac{-k^2}{4\beta^2}}}{(2\pi)^{\frac{3}{2}} k^2} \tag{10.23}$$

$$\phi(\mathbf{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \cdot \frac{4\pi}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} d^3k \frac{e^{\frac{-k^2}{4\beta^2}}}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{10.24}$$

$$\mathbf{k}\cdot\mathbf{r} = kr\cos\theta \tag{10.25}$$

$$\frac{d}{d\theta} e^{ikr\cos\theta} = -ikr\sin\theta e^{ikr\cos\theta} \tag{10.26}$$

$$\phi(\mathbf{r}) = \frac{4\pi}{8\pi^3} \int_0^{\infty} dk k^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \quad e^{ikr\cos\theta} \frac{e^{\frac{-k^2}{4\beta^2}}}{k^2} \tag{10.27}$$

$$= \frac{1}{2\pi^2} \cdot 2\pi \int_0^{\infty} dk \quad e^{\frac{-k^2}{4\beta^2}} \quad \underbrace{\left[\frac{e^{ikr\cos\theta}}{-ikr} \bigg|_0^{\pi} \right]}_{\frac{e^{-ikr}}{-ikr} + \frac{e^{ikr}}{ikr} = \frac{2\sin(kr)}{kr}}$$

$$= \frac{2}{\pi} \frac{1}{r} \int_0^{\infty} dk \frac{e^{\frac{-k^2}{4\beta^2}}}{k} \sin(kr)$$

$$= \frac{1}{r} \cdot \frac{2}{\pi} \cdot \frac{1}{2} (\pi \cdot 4\beta^2)^{\frac{1}{2}} \int_0^{r} dy \quad e^{-\beta^2 y^2}$$

let:

$$t = \beta y$$

$$dt = \beta dy = \frac{1}{r} \cdot \frac{2}{\pi} \cdot \frac{1}{2}\pi^{\frac{1}{2}} \cdot 2\beta \cdot \frac{1}{\beta} \int_0^{\beta r} dt \quad e^{-t^2}$$

$$\frac{erf(\beta r)}{r} \qquad \text{where} \qquad erf(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x dt \quad e^{-t^2}$$

Application:

$$g_\beta(\mathbf{r}) = \left(\frac{\beta}{\sqrt{\pi}}\right)^3 e^{-\beta^2 r^2} \qquad \int g_\beta(\mathbf{r}) d^3 r = 1$$

$$\begin{aligned} \widetilde{q}_\beta(\mathbf{k}) =& \frac{1}{(2\pi)^{\frac{3}{2}}} \cdot \int_{-\infty}^{\infty} d^3 r \left(\frac{\beta}{\sqrt{\pi}}\right)^3 e^{-\beta^2 r^2} e^{-i\mathbf{k}\cdot\mathbf{r}} \\ =& \frac{1}{(2\pi)^{\frac{3}{2}}} \cdot \left(\frac{\beta}{\sqrt{\pi}}\right)^3 \int_{-\infty}^{\infty} d^3 r e^{-(\beta\mathbf{r} - i\frac{\mathbf{k}}{2\beta})^2} e^{-\frac{k^2}{4\beta^2}} \end{aligned} \tag{10.28}$$

Since:

$$\left(\beta\mathbf{r} - i\frac{\mathbf{k}}{2\beta}\right)^2 = \beta^2 r^2 - 2i\beta\mathbf{r} \cdot \frac{\mathbf{k}}{2\beta} - \frac{k^2}{4\beta^2} \tag{10.29}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-\frac{k^2}{4\beta^2}} \underbrace{\left(\frac{\beta}{\sqrt{\pi}}\right)^3 \int_{-\infty}^{\infty} d^3 r' e^{-\beta^2 \cdot r'^2}}_{1} \qquad \mathbf{r}' = \mathbf{r} - \frac{i\mathbf{k}}{2\beta^2}$$

$$= \frac{e^{-\frac{k^2}{4\beta^2}}}{(2\pi)^{\frac{3}{2}}}$$

Note:

$$F_k\{\frac{1}{r}\} = \frac{(2\pi)^{\frac{3}{2}}}{k^2} \tag{10.30}$$

So

$$\begin{aligned} \widetilde{\phi}(\mathbf{k}) =& \frac{1}{(2\pi)^{\frac{3}{2}}} \cdot \frac{(2\pi)^{\frac{3}{2}}}{k^2} \frac{e^{-\frac{k^2}{4\beta^2}}}{(2\pi)^{\frac{3}{2}}} \\ =& \frac{e^{-\frac{k^2}{4\beta^2}}}{(2\pi)^{\frac{3}{2}} k^2} \end{aligned} \tag{10.31}$$

for a Gaussian $\widetilde{g_\beta(\mathbf{r})}$

Chapter 11

Ewald Sums

11.1 Rate of Change of a Vector

$$\underbrace{(d\mathbf{G})_s}_{\text{(space)}} = \underbrace{(d\mathbf{G})_{\text{body}}}_{\text{(body "r")}} + \underbrace{(d\mathbf{G})_{\text{rotational}}}_{\text{(rotational)}} = (d\mathbf{G})_{\text{r}} + d\mathbf{\Omega} \times \mathbf{G}$$

$$\left(\frac{d}{dt}\right)_s = \left(\frac{d}{dt}\right)_r + \boldsymbol{\omega} x \qquad \text{rotating coordinate system} \tag{11.1}$$

$$\left(\frac{d}{dt}\mathbf{r}\right) = \left(\frac{d\mathbf{r}}{dt}\right)_r + \boldsymbol{\omega} \times \mathbf{r} \qquad \mathbf{v}_s = \mathbf{v}_r + \boldsymbol{\omega} \times \mathbf{r}$$

"Newton's equations" $\quad \mathbf{F}_s = m\mathbf{Q}_s = m\left(\frac{d}{dt}\mathbf{v}_s\right)_s$

$$\begin{aligned}
\mathbf{F} =& m \cdot \left[\left(\frac{d}{dt}\{\mathbf{v}_r + \boldsymbol{\omega} \times \mathbf{r}\}\right)_s\right] \\
=& m\left[\underbrace{\left(\frac{d\mathbf{v}_r}{dt}\right)_r}_{\mathbf{a}_r} + \boldsymbol{\omega} \times \mathbf{v}_r + \left(\frac{d}{dt}(\boldsymbol{\omega} \times \mathbf{r})\right)_r + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})\right] \\
=& m\mathbf{a}_r + m\left[\boldsymbol{\omega} \times \mathbf{v}_r + \boldsymbol{\omega} \times \mathbf{v}_r + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})\right] \\
=& m\mathbf{a}_r + 2m(\boldsymbol{\omega} \times \mathbf{v}_r) + m[\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})]
\end{aligned} \tag{11.2}$$

$$\mathbf{F} - 2m\underbrace{(\ \boldsymbol{\omega} \times \mathbf{v}_r\ )}_{\text{Coriolis effect}} - m\underbrace{[\ \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})\ ]}_{\text{Centrifugal force}} = \mathbf{F}_{eff} = m\mathbf{a}_r$$

(Only if $\boldsymbol{\omega} \times \mathbf{v}_r \neq 0$, so $\mathbf{v}_r = 0$ or $\mathbf{v}_r \parallel \boldsymbol{\omega}$), and Centrifugal force$\sim 0.3\%$ of gravitational force.

11.2 Rigid Body Equations of Motion

Inertia tensor: $\mathbf{I}(3 \times 3)$

$$I_{jk} = \int_v \rho(\mathbf{r})(r^2\delta_{jk} - x_j x_k)d^3r \tag{11.3}$$

$$x_i = x, y, z \qquad \text{for } i = 1, 2, 3$$

e.g. for a system of point particles

$$I_{jk} = \sum_i m_i (r_i^2 \delta_{jk} - x_j x_k) \tag{11.4}$$

Note: Typically the origin is taken to be the center of mass.

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c}$$

$\mathbf{L} = \mathbf{I}\boldsymbol{\omega}$

$$\begin{aligned}
\mathbf{L} &= \sum_i \mathbf{r}_i \times \mathbf{p}_i \\
&= \sum_i m_i (\mathbf{r}_i \times \mathbf{v}_i) & \mathbf{v}_i &= \boldsymbol{\omega} \times \mathbf{r}_i \\
&= \sum_i m_i (\mathbf{r}_i \times (\boldsymbol{\omega} \times \mathbf{r}_i)) \\
&= \sum_i m_i [\boldsymbol{\omega} r_i^2 - \mathbf{r}_i (\mathbf{r}_i \cdot \boldsymbol{\omega})] \\
&= \sum_i \underbrace{[m_i r_i^2 \overleftrightarrow{1} - \mathbf{r}_i \mathbf{r}_i]}_{\overleftrightarrow{I} \text{ (old notation)}} \cdot \boldsymbol{\omega}
\end{aligned} \tag{11.5}$$

$$\begin{aligned}
T_r &= \sum_i \frac{1}{2} m_i v_i^2 \\
&= \sum_i \frac{1}{2} m_i \mathbf{v}_i \cdot \mathbf{v}_i \\
&= \sum_i \frac{1}{2} m_i \mathbf{v}_i \cdot (\boldsymbol{\omega} \times \mathbf{r}_i) \\
&= \sum_i \frac{1}{2} m_i \boldsymbol{\omega} \cdot (\mathbf{r}_i \times \mathbf{v}_i) \\
&= \frac{1}{2} \boldsymbol{\omega} \cdot \sum_i m_i (\mathbf{r}_i \times \mathbf{v}_i) \\
&= \frac{1}{2} \boldsymbol{\omega} \cdot \mathbf{L}
\end{aligned} \tag{11.6}$$

or

$$\begin{aligned}
T_r &= \frac{1}{2} \boldsymbol{\omega}^T \cdot \mathbf{I} \cdot \boldsymbol{\omega} \\
&= \frac{1}{2} I \omega^2
\end{aligned} \tag{11.7}$$

where $\boldsymbol{\omega} = \omega \mathbf{n}$ ($\mathbf{n} =$ axis of rotation) and $I = \mathbf{n}^T \cdot \mathbf{I} \cdot \mathbf{n}$

11.3 Principal Axis Transformation

$$\mathbf{U}\mathbf{T}\mathbf{U}^T = \mathbf{I}_D \qquad \text{(diagonal)} \qquad \mathbf{U}\cdot\mathbf{U}^T = \mathbf{1}$$

$$\mathbf{I}_D = \begin{pmatrix} I_{xx} & & 0 \\ & I_{yy} & \\ 0 & & I_{zz} \end{pmatrix}$$

I_{xx}, I_{yy}, and I_{zz} are the "principal moments" (eigenvalues) of $\mathbf{I}$.

Radius of gyration:

$$R_o = \frac{1}{m}\sum_i m_i r_i^2 \tag{11.8}$$

$$\text{or} \quad \frac{1}{m}\int \rho(\mathbf{r})\cdot r^2 d^3r \tag{11.9}$$

$$\text{or} \quad \sqrt{\frac{I}{m}} \tag{11.10}$$

$$\text{or} \quad \frac{1}{\mathbf{n}^T\cdot\boldsymbol{\rho}\sqrt{m}} \tag{11.11}$$

Moment of inertia about axis $\mathbf{n}$

$$\boldsymbol{\rho} = \mathbf{n}\cdot\frac{1}{\sqrt{I}} \tag{11.12}$$

$$I = \mathbf{n}^T\cdot\mathbf{I}\cdot\mathbf{n} \tag{11.13}$$

$$1 = \boldsymbol{\rho}^T\cdot\mathbf{I}\cdot\boldsymbol{\rho} \tag{11.14}$$

11.4 Solving Rigid Body Problems

$$T = \frac{1}{2}Mv^2 + \frac{1}{2}I\omega^2 = T_t + T_r$$

$$\begin{aligned} T_r &= \frac{1}{2}\boldsymbol{\omega}^T\cdot\mathbf{T}\cdot\boldsymbol{\omega} && \text{in general} \\ &= \frac{1}{2}\sum_i \omega_i I_{ii} && \text{in the principal axis system} \end{aligned} \tag{11.15}$$

11.5 Euler's equations of motion

$$\left(\frac{d\mathbf{L}}{dt}\right)_s = \left(\frac{d\mathbf{L}}{dt}\right)_r + \mathbf{w} \times \mathbf{L} = \underbrace{\mathbf{N}}_{\text{torque}} \tag{11.16}$$

$$\text{“space”} \qquad \text{“body”} \tag{11.17}$$

$$\text{system} \qquad \text{rotating system} \tag{11.18}$$

Recall:

$$\left(\frac{d}{dt}\right)_s = \left(\frac{d}{dt}\right)_b + \boldsymbol{\omega} x \tag{11.19}$$

In the principal axis system (which depends on time, since the body is rotating) takes the form:

$$I_i \frac{d\omega_i}{dt} + \epsilon_{ijk}\omega_j\omega_k I_k = N_i \tag{11.20}$$

$$I_i\dot{\omega}_i - \omega_j\omega_k(I_j - I_k) = N_i \tag{11.21}$$

$$i, j, k = 1, 2, 3 \quad 3, 1, 2 \quad 2, 3, 1$$

11.6 Torque-Free Motion of a Rigid Body

$$\left(\frac{d\mathbf{L}}{dt}\right)_{\mathbf{r}} + \boldsymbol{\omega} \times \mathbf{L} = \mathbf{N} = 0 \tag{11.22}$$

Example: Symmertical ($I_1 = I_2$) rigid body motion.

$$\left\{\begin{array}{l} I_1\dot{\omega}_1 = \omega_2\omega_3(I_2 - I_3) \\ I_2\dot{\omega}_2 = \omega_3\omega_1(I_3 - I_1) \\ I_3\dot{\omega}_3 = \omega_1\omega_2(I_1 - I_2) \end{array}\right. \xrightarrow{I_1 = I_2} \left.\begin{array}{c} I_1\dot{\omega}_1 = (I_1 - I_3)\omega_2\omega_3 \\ I_1\dot{\omega}_2 = (I_3 - I_1)\omega_1\omega_3 \\ I_3\dot{\omega}_3 = 0 \end{array}\right\}$$

$$I_3\dot{\omega}_3 = 0 \qquad\qquad I_3\omega_3 = L_3 = \text{ constant}$$

$$\dot{\boldsymbol{\omega}} = \boldsymbol{\omega} \times \boldsymbol{\Omega} \qquad\qquad \boldsymbol{\Omega} = \Omega\hat{z}_1$$

$$\dot{\omega}_1 = \frac{(I_1 - I_3)}{I_1}\omega_2\omega_3 = -\Omega\omega_2 \tag{11.23}$$

$$\dot{\omega}_2 = \Omega\omega_1 \tag{11.24}$$

where:

$$\Omega = \left(\frac{I_3 - I_1}{I_1}\right)\omega_3$$

Note: $\dot{\Omega} = 0$ since $\omega_3 = $ constant

$$\ddot{\omega}_1 = -\Omega^2\dot{\omega}_2 = \Omega\omega_1 \qquad \text{Harmonic!} \qquad \omega_1 = A\cos\Omega t$$
$$\ddot{\omega}_2 = \Omega\dot{\omega}_1 = -\Omega^2 \cdot A\sin\Omega t \qquad (\dot{\omega}_1 = -\Omega A\sin\Omega t)$$

So:

$$\omega_2 = A\sin\Omega t$$

Note:

$$\omega_1^2 + \omega_2^2 = A^2[\cos^2\Omega t + \sin^2\Omega t] = A^2 = \text{ constant}$$

This is an equation for a circle. Thus $\boldsymbol{\omega} =$ constant, $\omega_3 =$ constant, and $\boldsymbol{\omega}$ precesses around z axis with

11.7 Precession of a System of Charges in a Magnetic Field

$$\mathbf{m} = \frac{1}{2}\sum_i q_i(\mathbf{r}_i \times \mathbf{v}_i) \qquad \text{magnetic moment}$$

$$\mathbf{L} = \sum_i m_i(\mathbf{r}_i \times \mathbf{v}_i) \tag{11.25}$$

Consider the case when:

$$\mathbf{m} = \gamma\mathbf{L} \qquad \gamma = \frac{q}{2m} \quad \text{(gyromagnetic ratio)}$$

Example ↑ but γ often left unspecified.

$$V = -(\mathbf{m}\cdot\mathbf{B}) \qquad \mathbf{B} = \text{magnetic field} \tag{11.26}$$

$$\mathbf{N} = \mathbf{M}\times\mathbf{B} \qquad \text{(torque)} = \gamma\mathbf{L}\times\mathbf{B}$$

$$\begin{aligned}\left(\frac{d\mathbf{L}}{dt}\right)_s &= \gamma\mathbf{L}\times\mathbf{B} \\ &= \mathbf{L}\times(\gamma\mathbf{B})\end{aligned} \tag{11.27}$$

Same as $\left(\frac{d\mathbf{L}}{dt}\right)_r + \boldsymbol{\omega}\times\mathbf{L} = 0$ or $\left(\frac{d\mathbf{L}}{dt}\right)_r = \mathbf{L}\times\boldsymbol{\omega}$ (formula for torque free motion!)

$$\begin{aligned}\boldsymbol{\omega} &= -\frac{q}{2m}\mathbf{B} = \text{Larmor frequency} \\ &= \gamma\mathbf{B} \quad \text{(more general)}\end{aligned}$$

11.8 Derivation of the Ewald Sum

$$E = \sum_{i<j} q_i q_j r_{ij}^{-1}$$
$$= \frac{1}{2} \sum_i \sum_{j \neq i} q_i q_j r_{ij}^{-1}$$

$$\text{analogous} \quad \rightarrow \quad \frac{1}{2} \int \int \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) r_{12}^{-1} d\mathbf{r}_1 d\mathbf{r}_2$$

For periodic systems:

$$E = \frac{1}{2} \sum_i \sum_j q_i q_j \sum_{\mathbf{n}}{}' |\mathbf{r}_{ij} + \mathbf{n}|^{-1} \tag{11.28}$$
$$= \frac{1}{2} \sum_i \sum_j q_i q_j \Psi_E(\mathbf{r}_{ij})$$
$$= \frac{1}{2} \sum_i q_i \varphi(\mathbf{r}_i) \quad \text{where} \quad \varphi(\mathbf{r}_i) = \sum_j q_j \Psi_E(\mathbf{r}_{ij})$$

Consider the split:

$$\varphi(\mathbf{r}_i) = [\varphi(\mathbf{r}_i) - \varphi_s(\mathbf{r}_i)] + \varphi_s(\mathbf{r}_i)$$

$\varphi =$ potential of charges
$\varphi_s =$ “screening” of potential

For example, choose φ_s to come from a sum of spherical Gaussian functions:

$$g_\beta(\mathbf{r}) = \left(\frac{\beta}{\sqrt{\pi}} \right)^3 e^{-(\beta r)^2} \tag{11.29}$$

$$\rho_s(\mathbf{r}) = \sum_j q_j \sum_{\mathbf{n}} g_\beta(\mathbf{r} + \mathbf{n} - \mathbf{R}_j) \tag{11.30}$$

Note ρ_s is a smooth periodic function.

$$\nabla^2 \varphi_s(\mathbf{r}) = -4\pi \rho_s(\mathbf{r}) \tag{11.31}$$

11.9 Coulomb integrals between Gaussians

$$\int \int g_\alpha(\mathbf{r}_1 - \mathbf{R}_A) g_\beta(\mathbf{r}_2 - \mathbf{R}_B) r_{12}^{-1} d\mathbf{r}_1 d\mathbf{r}_2 \tag{11.32}$$
$$= \frac{erf\left[\frac{\alpha\beta}{\sqrt{\alpha^2+\beta^2}} R_{AB} \right]}{R_{AB}}$$

where:

$$erf(x) - \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

1. $\lim_{\alpha \to \infty}, \frac{erf(\beta R_{AB})}{R_{AB}}$

2. $\lim_{\alpha\to\beta}, \frac{erf\left[\left(\frac{\beta}{\sqrt{2}}\right)R_{AB}\right]}{R_{AB}}$

$$\begin{aligned}\varphi_{\text{real}}(\mathbf{r}_i) =&\varphi(\mathbf{r}_i) - \varphi_s(\mathbf{r}_i) \\ =&\sum_j q_j \sum_{\mathbf{n}}{}' \left(\frac{1}{|\mathbf{r}_{ij}+\mathbf{n}|} - \frac{erf(\beta|\mathbf{r}_{ij}+\mathbf{n}|)}{|\mathbf{r}_{ij}+\mathbf{n}|}\right) \\ =&\sum_j q_j \sum_{\mathbf{n}} \frac{erfc(\beta|\mathbf{r}_{ij}+\mathbf{n}|)}{|\mathbf{r}_{ij}+\mathbf{n}|}\end{aligned} \tag{11.33}$$

Short-ranged and can be altervated by β
One can choose β s.t. only the $\mathbf{n} = 0$ term is significant.

$$\varphi_{\text{real}}(\mathbf{r}_i) = \sum_{j\neq i} q_j \frac{erfc(\beta r_{ij})}{r_{ij}} - \underbrace{q_i\frac{\beta}{\sqrt{\pi}}}_{\text{“self term”}}$$

and Energy contribution

$$E_{\text{real}} = \frac{1}{2}\sum_i\sum_j q_i q_j \left(\frac{erfc(\beta r_{ij})}{r_{ij}} - \frac{2}{\sqrt{\pi}}\beta\delta_{ij}\right) \tag{11.34}$$

This choice of β is sometimes termed the “minimum image” β, and leads to a $\sigma(N^2)$ procedure for the real space term.

11.10 Fourier Transforms

For a periodic system described by lattice vectors:

$$\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

The Fourier transform must be taken over a reciprocal lattice.

$$\mathbf{m} = m_1\mathbf{a}_1^* + m_2\mathbf{a}_2^* + m_3\mathbf{a}_3^*$$

where the reciprocal space lattice vectors satisfy:

$$\mathbf{a}_i^* \cdot \mathbf{a}_j = \delta_{ij} \qquad i, j = 1, 2, 3$$

or

$$\mathbf{PQ} = \mathbf{1} = \mathbf{QP} \qquad\qquad \mathbf{Q} = \mathbf{P}^{-1}$$

$$\mathbf{P} = (\mathbf{a}_1 \quad \mathbf{a}_2 \quad \mathbf{a}_3)$$

$$\dot{\mathbf{Q}} = \begin{pmatrix}\mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^*\end{pmatrix}$$

$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \times \mathbf{a}_2 \cdot \mathbf{a}_3} = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{v} = \mathbf{f}(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \tag{11.35}$$

$$\mathbf{a}_1^* = \mathbf{f}(\mathbf{a}_3, \mathbf{a}_1, \mathbf{a}_2) \quad \} \tag{11.36}$$

$$\mathbf{a}_1^* = \mathbf{f}(\mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_1) \quad \} \qquad \text{cyclic permutation} \tag{11.37}$$

$$\tag{11.38}$$

The discrete Fourier transform representation of a function over the reciprocal lattice is:

$$f(\mathbf{r}) = \frac{1}{v} \sum_{\mathbf{k}}^{\infty} \hat{f}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{11.39}$$

where:

$$\mathbf{k} = 2\pi\mathbf{m} = 2\pi(m_1\mathbf{a}_1^* + m_2\mathbf{a}_2^* + m_3\mathbf{a}_3^*)$$

We now return to:

1. $\nabla^2 \varphi_s(\mathbf{r}) = -4\pi\rho_s(\mathbf{r})$

where

$$\rho_s(\mathbf{r}) = \sum_j q_j g_\beta(\mathbf{r} - \mathbf{R}_j) \tag{11.40}$$

Note:

$$F\{g_\beta(\mathbf{r})\} = e^{-\frac{k^2}{4\beta^2}} \tag{11.41}$$

Fourier transform of 1. gives:

$$(i\mathbf{k})^2 \widetilde{\varphi}_s(\mathbf{k}) = -4\pi\widetilde{\rho}_s(\mathbf{k}) \tag{11.42}$$

$$\widetilde{\varphi}_s(\mathbf{k}) = 4\pi \frac{\widetilde{\rho}_s(\mathbf{k})}{k^2} \tag{11.43}$$

by inverse transforming we obtain:

$$\varphi(\mathbf{r}) = \frac{1}{v} \sum_j \sum_k q_j 4\pi \frac{e^{-\frac{k^2}{4\beta^2}}}{k^2} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_j)} \tag{11.44}$$

Note: this blows up at $\mathbf{k} = 0$! Can we throw this term out?

$$\varphi_s(\mathbf{r}) = \frac{1}{v} \sum_{\mathbf{k}} 4\pi \frac{\widetilde{\rho}(\mathbf{k})}{k^2} \tag{11.45}$$

but $\widetilde{\rho}_s(0) = \int \rho_s(\mathbf{r}) d\mathbf{r} = 0$ for neutral system!

It turns out we can throw out the $\mathbf{k} = 0$ term if:

1. system is neutral
2. system has no dipole moment

Under these conditions we have:

$$\varphi_s(\mathbf{r}) = \frac{4\pi}{v}\sum_{\mathbf{k}\neq 0}\frac{\widetilde{\rho}_s(\mathbf{k})}{k^2} \tag{11.46}$$

If there is a dipole, an extra term in the energy must be added of the form:

$$J(P,\mathbf{D},E) \propto |\dot{D}|^2$$

$$\begin{aligned} \mathbf{D} &= \text{dipole} \\ P &= \text{shape} \\ E &= \text{dielectric} \end{aligned}$$

What do we do in solution?
(What "errors" are introduced due to periodicity?)

11.11 Linear-scaling Electrostatics

$$\begin{aligned} E =& \frac{1}{2}\int \rho(\mathbf{r})\phi(\mathbf{r})d^3r \\ =& \frac{1}{2}\int\int \rho(\mathbf{r})G(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}')d^3r'd^3r \end{aligned} \tag{11.47}$$

$$\phi(\mathbf{r}) = \int G(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}')d^3r' \tag{11.48}$$

$$\begin{aligned} \nabla^2\phi(\mathbf{r}) = -4\pi\rho(\mathbf{r}) \quad &\leftarrow \quad \epsilon(\mathbf{r}) = 1 \text{ "gas-phase"} \\ \nabla^2 G(\mathbf{r},\mathbf{r}') = -4\pi\delta(\mathbf{r},\mathbf{r}') \end{aligned}$$

$$G(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|} \qquad \text{(non periodic)} \tag{11.49}$$

$$\frac{4\pi}{v}\sum_{\mathbf{k}=0}^{\infty}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2} \qquad \text{(periodic)} \tag{11.50}$$

$$(\mathbf{k} = 2\pi\mathbf{m})$$

11.12 Green's Function Expansion

$$G(\mathbf{r},\mathbf{r}') = \sum_k N_k(\mathbf{r})M_k(\mathbf{r}') \tag{11.51}$$

Seperable!

11.13 Discrete FT on a Regular Grid

$$\begin{aligned} f(x) \to f(x_n) = f_n \qquad & x_n = n\Delta \qquad & n = o, \ldots N-1 \\ \hat{f}(k) \to \hat{f}(k_m) = \hat{f}_m \qquad & k_m = \frac{2m\pi}{N\Delta} \qquad & m = -\frac{N}{2}, \ldots 0, \ldots \frac{N}{2} \end{aligned} \tag{11.52}$$

$$\hat{f}_{(k)} = \int f(x) e^{ikx} dx \approx \sum_{n=o}^{N-1} f_n e^{i2\pi \frac{mn}{N}} = \hat{f}_m \tag{11.53}$$

similarly

$$f_n = \frac{1}{N} \sum_{m=0}^{N-1} f_m e^{-i2\pi \frac{mn}{N}} \tag{11.54}$$

11.14 FFT

Danielson-Lanczos Lemma

$$W_N \equiv e^{\frac{i2\pi}{N}} \tag{11.55}$$

$$f_m = \sum_{n=0}^{N-1} W_N^{nm} f_n \tag{11.56}$$

$$\begin{aligned} &= \sum_{n=0}^{\frac{N}{2}-1} W_{\frac{N}{2}}^{nm} f_{2n} + W_N^m \sum_{n=0}^{\frac{N}{2}-1} W^{nm} f_{2n+1} \\ &= F_m^e + W_N^m f_m^o \to \text{ 2 FT's of dim. } \frac{N}{2} \end{aligned} \tag{11.57}$$

Used recursively with “bit reversal” to obtain the full FFT in $\sigma(N \log N)$!

Ewald Sums (Linear Scaling)

$$\rho(\mathbf{r}) = \sum_i q_i \delta(\mathbf{r} - \mathbf{R}_i) \tag{11.58}$$

$$\rho_s(\mathbf{r}) = \sum_i q_i g(\mathbf{r} - \mathbf{R}_i) \tag{11.59}$$

$$\text{e.g.} \qquad g(\mathbf{r}) = \left(\frac{\beta}{\sqrt{\pi}}\right)^3 e^{-\beta^2 r^2}$$

$$\rho(\mathbf{r}) = [\rho(\mathbf{r}) - \rho_s(\mathbf{r})] + \rho_s(\mathbf{r}) \tag{11.60}$$

$$\phi(\mathbf{r}) = [\phi(\mathbf{r}) - \phi_s(\mathbf{r})] + \phi_s(\mathbf{r}) \tag{11.61}$$

$$\nabla^2 \phi_s(\mathbf{r}) = -4\pi\rho_s(\mathbf{r}) \tag{11.62}$$

Fourier transform

$$-k^2 \widetilde{\phi}_s(\mathbf{k}) = -4\pi\widetilde{\rho}_s(\mathbf{k}) \tag{11.63}$$

Particle-Mesh, P^3M Methods

FFT $g(\mathbf{r})$, $\sum_i q_i \delta(\mathbf{r} - \mathbf{R}_i)$ to obtain $\widetilde{\rho}_s(\mathbf{k})$

Note: $\widetilde{\rho}_s(\mathbf{k})$ is the transform of $\rho_s(\mathbf{r})$ (a plane wave expansion)

11.15 Fast Fourier Poisson

Evaluate $\rho_2(\mathbf{r})$ directly on grid. (No interpolation)

Solve for $\phi_s(\mathbf{r})$ on grid. Modify real space term accordingly.

$$\begin{aligned} E =& \frac{1}{2} \sum_i \sum_{j \neq i} q_i q_j \frac{erfc(\beta' r_{ij})}{r_{ij}} \\ & - \sum_i q_i^2 \frac{\beta'}{\sqrt{\pi}} \\ & + \underbrace{\frac{1}{2} \int \rho_s(\mathbf{r}) \phi_s(\mathbf{r}) d^3 r}_{\frac{1}{2}\sum_{ijk} \rho_s(i,j,k)\phi_s(i,j,k)} + J(\mathbf{D}, P, \epsilon) \end{aligned} \tag{11.64}$$

$$\beta' = \frac{\beta}{\sqrt{2}}$$

which equals the exact integral for the plane-wave projected density.

Chapter 12

Dielectric

12.1 Continuum Dielectric Models

Gas phase:

$$\nabla^2\phi_o(\mathbf{r}) = -4\pi\rho_o(\mathbf{r}) \qquad \phi_o(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r'$$

$$\nabla \cdot \mathbf{E}_o = 4\pi\rho_o$$

Suppose in addition to $\rho_o(\mathbf{r})$ there is a dipole polarization $\mathbf{p}(\mathbf{r})$, then:

$$\begin{aligned}
\phi(\mathbf{r}) &= \int \left(\frac{\rho_o(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \frac{\mathbf{P}(\mathbf{r}')\cdot(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3} \right) d^3r \\
&= \int \left(\frac{\rho_o(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \mathbf{P}(\mathbf{r}')\nabla_{r^{-1}} \left(\frac{1}{|\mathbf{r}-\mathbf{r}'|} \right) \right) d^3r' \\
&= \int \left(\frac{\rho_o(\mathbf{r}') - \nabla_{\mathbf{r}^{-1}} \cdot \mathbf{P}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \right) d^3r' \\
&= \int \left(\frac{\rho_o(\mathbf{r}') + \sigma_{pol}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \right) d^3r' \\
&= \frac{1}{4\pi} \int \left(\frac{\nabla_{\mathbf{r}^{-1}} \cdot (\mathbf{E}_o(\mathbf{r}') - 4\pi\mathbf{P}(\mathbf{r}'))}{|\mathbf{r}-\mathbf{r}'|} \right) d^3r' \\
&\qquad [\sigma_{pol}(\mathbf{r}) = -\nabla_{\mathbf{r}} \cdot \mathbf{P}(\mathbf{r})]
\end{aligned} \tag{12.1}$$

$$\begin{aligned}
\nabla^2\phi(\mathbf{r}) &= -\boldsymbol{\nabla}\cdot\mathbf{E}(\mathbf{r}) \\
&= -4\pi(\rho_o(\mathbf{r}) + \sigma_{pol}(\mathbf{r}))
\end{aligned} \tag{12.2}$$

$$\mathbf{D}(\mathbf{r}) \equiv \mathbf{E}(\mathbf{r}) + 4\pi\boldsymbol{\rho}(\mathbf{r}) \tag{12.3}$$

$$\begin{aligned}
\boldsymbol{\nabla}\cdot\mathbf{D} &= \boldsymbol{\nabla}\cdot\mathbf{E} + 4\pi\boldsymbol{\nabla}\cdot\boldsymbol{\rho} \\
&= 4\pi\rho_o + 4\pi\sigma_{pol} - 4\pi\sigma_{pol} \\
&= 4\pi\rho_o
\end{aligned} \tag{12.4}$$

$$\boldsymbol{\nabla} \cdot \mathbf{D} = 4\pi\rho_o$$

So where does $\boldsymbol{\rho}$ come from?

$$\boldsymbol{\rho} = x_e \cdot \mathbf{E} \qquad x_e = \text{electric susceptibility}$$

$$\mathbf{D} = \mathbf{E} + 4\pi\boldsymbol{\rho} = (1 + 4\pi x_e)\mathbf{E} = \epsilon\mathbf{E} \qquad \text{(LPIM)}$$

$$\epsilon(\mathbf{r}) \equiv 1 + 4\pi x_e \qquad \text{static dielectric function}$$

$$\begin{aligned} \nabla \cdot \mathbf{D} =& 4\pi\rho_o \\ =& \nabla \cdot (\epsilon\mathbf{E}) \\ =& 4\pi\rho_o \end{aligned} \tag{12.5}$$

$$\nabla(\epsilon\nabla\phi) = -4\pi\rho_o \qquad \text{Poisson equation for lin. isotropic pol. med.}$$

$$\phi(\mathbf{r}) = \phi_o(\mathbf{r}) + \phi_{pol}(\mathbf{r}) \tag{12.6}$$

$$\nabla \cdot \epsilon(\nabla\phi_o + \nabla\phi_{pol}) = -4\pi\rho_o \tag{12.7}$$

$$\nabla\epsilon \cdot \nabla(\phi_o + \phi_{pol}) + \underbrace{\epsilon\nabla^2\phi_o}_{-\epsilon 4\pi\rho_o} + \epsilon\nabla^2\phi_{pol} = -4\pi\rho_o \tag{12.8}$$

$$\epsilon\nabla^2\phi_{pol} = -4\pi\rho_o[1 - \epsilon] - \nabla\epsilon \cdot \nabla\phi \tag{12.9}$$

$$\begin{aligned} \nabla^2\phi_{pol} =& -4\pi\rho_o\frac{[1 - \epsilon]}{\epsilon} - \frac{\nabla\epsilon}{\epsilon} \cdot \nabla\phi \\ =& -4\pi\sigma_{pol} \end{aligned} \tag{12.10}$$

12.2 Gauss' Law I

$$
\begin{aligned}
\int_{v=\infty} \sigma_{pol}(\mathbf{r}) d^3r &= \int \rho_o \left(\frac{1-\epsilon}{\epsilon}\right) d^3r + \frac{1}{4\pi}\int \frac{\nabla\epsilon}{\epsilon}\cdot\nabla\phi d^3r \qquad (12.11)\\
&= \int \rho_o \left(\frac{1}{\epsilon}-1\right) d^3r + \frac{1}{4\pi}\int \nabla\left(\frac{1}{\epsilon}\right)\cdot\epsilon\mathbf{E} d^3r\\
&= \int \rho_o \left(\frac{1}{\epsilon}-1\right) d^3r - \frac{1}{4\pi}\int \left(\frac{1}{\epsilon}\right)\nabla\cdot\mathbf{D} d^3r + \frac{1}{4\pi}\int_{s=\infty}\left(\frac{1}{\epsilon}\right)\mathbf{D}\cdot\hat{n}da\\
&= \int \rho_o \left(\frac{1}{\epsilon}-1-\frac{1}{\epsilon}\right) d^3r + \frac{1}{4\pi}\int_{s=\infty}\left(\frac{1}{\epsilon}\right)\mathbf{D}\cdot\hat{n}da\\
&= -\int \rho_o d^3r + \frac{1}{4\pi}\cdot\frac{1}{\epsilon_2}\int_{s=\infty}\mathbf{D}\cdot\hat{n}da\\
&= -\int \rho_o d^3r + \frac{1}{\epsilon\,2}\int \rho_o d^3r\\
&= \left(\frac{1-\epsilon_2}{\epsilon_2}\right)\int \rho_o d^3r
\end{aligned}
$$

$$\nabla\left(\frac{1}{\epsilon}\right) = -\frac{\nabla\epsilon}{\epsilon^2}$$

let $\epsilon \longrightarrow \epsilon_2$ are $s=\infty$ (constant). Note: $\int \mathbf{D}\cdot\hat{n}da = \int\nabla\cdot\mathbf{D}d^3r = 4\pi\int\rho_o d^3r$

$$\int_{v=\infty}\sigma_{pol}(\mathbf{r})d^3r = -\left(\frac{\epsilon_2-1}{\epsilon_2}\right)\int_{v=\infty}\rho_o(\mathbf{r})d^3r \qquad (12.12)$$

Gauss' Law I: Volume integral over all space.

If ϵ changes from ϵ_1 to ϵ_2 discontinuously at a dielectric boundary defining the surface s_{12}, then care must be taken to insure the boundary conditions.

$(\mathbf{D}_2-\mathbf{D}_1)\cdot\hat{n}_{21} = 4\pi\sigma_o$ where σ_o is a static surface charge density (part of ρ_o)

$$(\mathbf{E}_2-\mathbf{E}_1)\times\hat{n}_{21} = 0 \qquad (12.13)$$

This implies:

$$\sigma_{pol} = -(\boldsymbol{\rho}_2-\boldsymbol{\rho}_1)\cdot\hat{n}_{21} \qquad (12.14)$$

where

$$
\begin{aligned}
\boldsymbol{\rho}_i &= \left(\frac{\epsilon_i-1}{4\pi}\right)\mathbf{E}_i \qquad (12.15)\\
&= \left(\frac{\epsilon_i-1}{4\pi\epsilon_i}\right)\mathbf{D}_i
\end{aligned}
$$

Recall:

$$\mathbf{D} = \mathbf{E} = 4\pi\boldsymbol{\rho} \qquad \boldsymbol{\rho} = \frac{1}{4\pi}(\mathbf{D}-\mathbf{E})$$

dielectric dicont. $\epsilon_1\epsilon_2$ and s_{12}

If $\sigma_o = 0$, $\mathbf{D}_2 \cdot \hat{n}_{21} = \mathbf{D}_1 \cdot \hat{n}_{21} = \mathbf{D} \cdot \hat{n}_{21}$

$$\begin{aligned}\sigma_{pol} &= -\left(\boldsymbol{\rho}_2 - \boldsymbol{\rho}_1\right) \cdot \hat{n}_{21} \\ &= -\left[\frac{\epsilon_2 - 1}{4\pi\epsilon_2}\boldsymbol{\rho}_2 - \frac{\epsilon_1 - 1}{4\pi\epsilon_1}\mathbf{D}_1\right] \cdot \hat{n}_{21} \\ &= -\frac{1}{4\pi}\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_2\epsilon_1}\right)\mathbf{D}\end{aligned} \tag{12.16}$$

12.3 Gauss' Law II

$$\sigma_{pol} = -\frac{1}{4\pi}\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_2\epsilon_1}\right)\mathbf{D} \cdot \hat{n}_{21} \tag{12.17}$$

$$\begin{aligned}\int_{s_{12}} \sigma_{pol} da &= -\frac{1}{4\pi}\int_{s_{12}}\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_1\epsilon_2}\right)\mathbf{D} \cdot \hat{n}_{21} da \\ &= -\frac{1}{4\pi}\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_1\epsilon_2}\right)\int_{v_1} \nabla \cdot \mathbf{D} d^3r \\ &= -\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_1\epsilon_2}\right)\int_{v_1} \rho_o d^3r \\ &= -\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_1\epsilon_2}\right) Q_o(v_1)\end{aligned} \tag{12.18}$$

$$\int_{s_{12}} \sigma_{pol} da = -\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_1\epsilon_2}\right) Q_o(v_1) \tag{12.19}$$

Guass' Law II for integral over surface at dielectric discontinuity.

12.4 Variational Principles of Electrostatics

Electrostatic energy:

$$W = \frac{1}{4\pi}\int d^3r \int_0^{\mathbf{D}} \mathbf{E} \cdot \delta\mathbf{D} \qquad \text{(Nonlinear dielectric medium)} \tag{12.20}$$

if medium is linear, $\int_0^{\mathbf{D}} \mathbf{E} \cdot \delta\mathbf{D} = \frac{1}{2}\mathbf{E} \cdot \mathbf{D}$, then:

$$\begin{aligned}W =& \frac{1}{8\pi}\int d^3r \mathbf{E} \cdot \mathbf{D} \\ =& \frac{1}{8\pi}\int d^3r (-\nabla\phi) \cdot \mathbf{D} \\ =& \frac{1}{4\pi}\int d^3r \phi \nabla \cdot \mathbf{D} - \frac{1}{4\pi}\int_{s=\infty} \phi \mathbf{D} \cdot \hat{n} da \\ =& \frac{1}{2}\int d^3r \rho_o \phi\end{aligned} \tag{12.21}$$

$$W[\phi, \rho_o, \epsilon] \equiv \int \rho_o(\mathbf{r})\phi(\mathbf{r}) d^3r - \frac{1}{8\pi}\int \nabla\phi \cdot \epsilon \cdot \nabla\phi d^3r \tag{12.22}$$

$$\frac{\delta W}{\delta \phi(\mathbf{r})} = \rho_o(\mathbf{r}) + \frac{2}{8\pi}\nabla\cdot[\epsilon\nabla\phi] = 0 \tag{12.23}$$

$$\nabla\cdot[\epsilon\nabla\phi] = -4\pi\beta \qquad \text{(The Poisson equation with dielectric)}$$

The variational prinicple allows ϕ to be solved for using optimization methods. Do you minimize or maximize?

$$\frac{\delta W}{\delta \phi(\mathbf{r})} = \rho_o(\mathbf{r}) + \frac{1}{4\pi}\nabla\cdot[\epsilon\nabla\phi] \tag{12.24}$$

$$= \int d^3r' \left[\rho_o(\mathbf{r}) + \frac{1}{4\pi}\nabla_{\mathbf{r}'}[\epsilon(\mathbf{r})\nabla_{\mathbf{r}'}\phi(\mathbf{r}')]\right]\delta(\mathbf{r}-\mathbf{r}')d^3r'$$

$$\frac{\delta^2 W}{\delta\phi(\mathbf{r})\delta\phi(\mathbf{r}')} = \frac{1}{4\pi}\nabla_{\mathbf{r}'}\cdot[\epsilon(\mathbf{r}')\nabla_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}')] \tag{12.25}$$

if $\epsilon > D$, the operator is negative in that:

$$\int\int f(\mathbf{r})\frac{\delta^2 W}{\delta\phi(\mathbf{r})\delta\phi(\mathbf{r})}f(\mathbf{r}')d^3rd^3r' = \int\int f(\mathbf{r})\nabla_{\mathbf{r}'}\cdot[\epsilon(\mathbf{r}')\nabla_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}')]f(\mathbf{r}')d^3rd^3r' \tag{12.26}$$

$$= -\int\int f(\mathbf{r})[\epsilon(\mathbf{r}')\nabla_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}')]\cdot\nabla_{\mathbf{r}'}f(\mathbf{r}')d^3rd^3r'$$

$$= \int\int f(\mathbf{r})[\epsilon(\mathbf{r}')\nabla_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}')]\cdot\nabla_{\mathbf{r}}f(\mathbf{r}')d^3rd^3r'$$

$$= -\int \epsilon(\mathbf{r}')|\nabla f(\mathbf{r}')|^2 d^3r' \leq 0$$

hence $W[\phi]$ is maximized to obtain $\phi(\mathbf{r})$.

$$\epsilon = 1 \qquad W = [\phi,\rho_o,\epsilon=1] = \int \rho_o\phi d^3r - \frac{1}{8\pi}\int\nabla\phi\cdot\nabla\phi d^3r$$

12.5 Electrostatics - Recap

"Gas-phase" "in vacuo" "$\epsilon = 1$"

$$\nabla^2_{\mathbf{r}}\phi_o(\mathbf{r}) = -4\pi\rho(\mathbf{r}) \qquad (\hat{L}\phi = -4\pi\rho)$$

$$\phi_o(\mathbf{r}) = \int G_o(\mathbf{r},\mathbf{r}')\rho_o(\mathbf{r}')d^3r' \tag{12.27}$$

where:

$$\nabla_{\mathbf{r}^2}G_o(\mathbf{r},\mathbf{r}') = -4\pi\delta(\mathbf{r}-\mathbf{r}') \tag{12.28}$$

depends on boundary conditions:

$$G_o(\mathbf{r},\mathbf{r}') = \begin{cases} \frac{1}{|\mathbf{r}-\mathbf{r}'|} & \text{“real space”}\phi, \nabla\phi = 0, r\to\infty \\ \frac{4\pi}{v}\sum_{k=o}^{\infty}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2} & \mathbf{k} = 2\pi\mathbf{m} \\ & \mathbf{m} = m_1\mathbf{a}_1^* + m_2\mathbf{a}_2^* + m_3\mathbf{a}_3^* \end{cases}$$

Sometimes we can use the Green's function and analytically obtain a solution for the potential. In real space, for example Gaussian:

$$\rho_1(\mathbf{r}) = \left(\frac{\beta}{\sqrt{\pi}}\right)^3 e^{-(\beta_1|\mathbf{r}-\mathbf{R}_1|)^2} \qquad \rho_2(\mathbf{r}) = \left(\frac{\beta}{\sqrt{\pi}}\right)^3 e^{-(\beta_2|\mathbf{r}-\mathbf{R}_2|)^2}$$

$$\begin{aligned}\phi_1(\mathbf{r}) &= \int \frac{\rho_1(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r' \\ &= \frac{erf(\beta, r)}{r}\end{aligned} \tag{12.29}$$

$$\int\int \frac{\rho_1(\mathbf{r})\rho_2(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r d^3r' = \frac{erf(\beta'_{12}R_{12})}{R_{12}} \tag{12.30}$$

$$\beta'_{12} = \frac{\beta_1 \cdot \beta_2}{\sqrt{\beta_1^2 + \beta_2^2}} \tag{12.31}$$

In reciprocal space, Ewald sum:
For minimum image β'' s.t. $\mathbf{n} = 0$ only term.

$$\begin{aligned}E =& \frac{1}{2}\sum_i \sum_j q_i q_j \left(\frac{erfc(\beta r_{ij})}{r_{ij}} - \frac{\beta}{\sqrt{\pi}}\delta_{ij} + \frac{4\pi}{v}\sum_{\mathbf{k}=0} \frac{e^{-\frac{k^2}{4\beta^2}}}{k^2} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right) \\ =& \sum_i \sum_{j<i} q_i q_j \left(\frac{erfc(\beta r_{ij})}{r_{ij}} - \frac{\beta}{\sqrt{\pi}}\delta_{ij} \right) + \frac{2\pi}{v}\sum_{\mathbf{k}=0} \frac{e^{-\frac{k^2}{4\beta^2}}}{k^2} |s(\mathbf{k})|^2\end{aligned} \tag{12.32}$$

$$s(\mathbf{k}) = \sum_i q_i e^{i\mathbf{k}\cdot\mathbf{r}_i} \tag{12.33}$$

Sometimes, however, we need to break down $G_o(\mathbf{r}, \mathbf{r}')$ into a product form, and found it useful to expand $G(\mathbf{r}, \mathbf{r}')$ in terms of eigenvectors of it's associated operator. This leads to:
Real space:

$$\phi(\mathbf{r}) = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \sum_{m=-\ell}^{\ell} y_{\ell m} \overbrace{(\theta, \varphi)}^{\Omega} \phi_{\ell m}(r) \tag{12.34}$$

$$\phi_{\ell m}(r) = \frac{1}{r^{\ell+1}} \int_0^r x^{(2+\ell)} \rho_{\ell m}(x) dx + r^\ell \int_0^\infty x^{(1-\ell)} \rho_{\ell m}(x) dx \tag{12.35}$$

where

$$\rho_{\ell m}(r) = \int d\Omega y^*_{\ell m}(\Omega) \rho(\mathbf{r}) \tag{12.36}$$

or Fourier transforms:

$$-k^2 \widetilde{\phi}(\mathbf{k}) = -4\pi \widetilde{\rho}(\mathbf{k}) \tag{12.37}$$

$$\phi(\mathbf{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3k e^{i\mathbf{k}\cdot\mathbf{r}} \left(\frac{4\pi\widetilde{\rho}(\mathbf{k})}{k^2} \right) \tag{12.38}$$

$$\widetilde{\rho}(\mathbf{k}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3k \left(e^{i\mathbf{k}\cdot\mathbf{r}} \right)^* \rho(\mathbf{r}) \tag{12.39}$$

Reciprocal space (lattice):

$$\phi(\mathbf{r}) = \frac{4\pi}{v} \sum_{\mathbf{k}=0} \frac{\widetilde{\rho}(\mathbf{k})}{k^2} \tag{12.40}$$

for:

$$\mathbf{k} = 2\pi\mathbf{m} \qquad\qquad \mathbf{m} = \sum_{i=1}^{3} m_i \mathbf{a}_i^*$$

12.6 Dielectrics

$$\nabla \cdot \mathbf{D} = 4\pi\rho_o \tag{12.41}$$

$$\begin{aligned} \mathbf{D} &= \epsilon\mathbf{E} \\ &= \mathbf{E} + 4\pi\boldsymbol{\rho} \end{aligned} \tag{12.42}$$

$$\mathbf{E} = -\nabla\phi \tag{12.43}$$

Poisson equation for a linear isotropic polarizable medium characterized by $\epsilon(\mathbf{r})$

$$\nabla \cdot [\epsilon\nabla\phi] = -4\pi\rho_o \tag{12.44}$$

$$\sigma_{pol}(\mathbf{r}) \equiv -\nabla \cdot \boldsymbol{\rho} \tag{12.45}$$

$$\phi(\mathbf{r}) = \int \frac{(\rho_o(\mathbf{r}') = \sigma_{pol}(\mathbf{r}'))}{|\mathbf{r} - \mathbf{r}'|} d^3r' \tag{12.46}$$

$$\sigma_{pol}(\mathbf{r}) = \rho_o \frac{[1-\epsilon]}{\epsilon} + \frac{1}{4\pi}\frac{\nabla\epsilon}{\epsilon} \cdot \nabla\phi \tag{12.47}$$

Gauss Law I:

$$\int_{v=\infty} \sigma_{pol}(\mathbf{r}) d^3r = -\left(\frac{\epsilon_2 - 1}{\epsilon_2}\right) \int_{v=\infty} \rho_o(\mathbf{r}) d^3r \tag{12.48}$$

Gauss Law II:

$$\int_{s_{12}} \sigma_{pol}(\mathbf{r}) da = -\left(\frac{\epsilon_2 - \epsilon_1}{\epsilon_1\epsilon_2}\right) \int_{v_1} \rho_o(\mathbf{r}) d^3r \tag{12.49}$$

$$\begin{aligned} \rho_{ion}(\mathbf{r}) &= \sum_s c_s q_s e^{-\beta q_s \phi(\mathbf{r})} && (c_s = \text{conc.}) \\ &\approx \sum_s c_s q_s - \beta \sum_s -\beta \sum_s c_s q_s^2 \phi && \text{(linearized)} \end{aligned}$$

For Born ion, LPB equation leads to:

$$\nabla^2\phi - k^2\phi = -4\pi\rho_o(\mathbf{r}) \tag{12.50}$$

$$k^2 = \frac{4\pi\beta}{\epsilon}\sum_s q_s^2 c_s \tag{12.51}$$

(Note: $I = \frac{1}{2}\sum_s q_s^2 c_s$ ion conc.)

$$\phi(\mathbf{r}) = q_{ion}\frac{e^{-kr}}{\epsilon r} \qquad \text{(pt. chg.)} \tag{12.52}$$

or

$$\phi(\mathbf{r}) = \frac{q_{ion}e^{-k(r-a)}}{\epsilon r(1+ka)} \qquad \text{(ion of radius } a\text{)} \tag{12.53}$$

$$x^2_{E_{pol}}[\phi_{pol};\phi_o,\epsilon] = \frac{1}{2}\int\epsilon\Bigg[\underbrace{\mathbf{E}_{pol}}_{-\nabla\phi_{pol}} + \left(\frac{\epsilon-1}{\epsilon}\right)\underbrace{\mathbf{E}_o}_{-\nabla\phi_o}\Bigg]^2 d^3r \tag{12.54}$$

$$\frac{\delta x^2_{E_{pol}}}{\delta\phi_{pol}} = -\nabla\cdot\left[2\cdot\epsilon\left(\nabla\phi_{pol} + \left(\frac{\epsilon-1}{\epsilon}\right)\nabla\phi_o\right)\right] = 0 \tag{12.55}$$

$$\nabla\epsilon\cdot\left(\nabla\phi_{pol} + \frac{\epsilon-1}{\epsilon}\nabla\phi_o\right) + \epsilon\underbrace{\nabla^2\phi_{pol}}_{-4\pi\sigma_{pol}} + \epsilon\nabla\left(\frac{\epsilon-1}{\epsilon}\right)\cdot\nabla\phi_o + \epsilon_o + \epsilon\left(\frac{\epsilon-1}{\epsilon}\right)\underbrace{\nabla^2\phi_o}_{-4\pi\rho_o} = 0 \tag{12.56}$$

leads to:

$$\sigma_{pol} = -\left(\frac{\epsilon-1}{\epsilon}\right)\rho_o + \frac{1}{4\pi}\frac{\nabla\epsilon}{\epsilon}\cdot\nabla\phi \tag{12.57}$$

$\frac{1}{4\pi\epsilon}\times\rightarrow$

$$\sigma_{pol} = -\left(\frac{\epsilon-1}{\epsilon}\right)\rho_o + \frac{1}{4\pi}\frac{\nabla\epsilon}{\epsilon}\cdot\left(\nabla\phi_{pol} + \frac{\epsilon-1}{\epsilon}\nabla\phi_o\right) + \frac{1}{4\pi}\nabla\left(\frac{\epsilon-1}{\epsilon}\right)\cdot\nabla\phi_o \tag{12.58}$$

Note:

$$\begin{aligned}\nabla\left(\frac{\epsilon-1}{\epsilon}\right) &= \frac{\nabla\epsilon}{\epsilon} + (\epsilon-1)\nabla\left(\frac{1}{\epsilon}\right)\\ &= \frac{\nabla\epsilon}{\epsilon} - (\epsilon-1)\frac{\nabla\epsilon}{\epsilon^2}\\ &= \frac{\nabla\epsilon}{\epsilon^2}\end{aligned} \tag{12.59}$$

$$\frac{\nabla\epsilon}{\epsilon}\cdot\frac{(\epsilon-1)}{\epsilon} + \frac{\nabla\epsilon}{\epsilon^2} = \frac{\nabla\epsilon}{\epsilon} \tag{12.60}$$

$$\sigma_{pol} = -\left(\frac{\epsilon - 1}{\epsilon}\right)\rho_o + \frac{1}{4\pi}\frac{\nabla\epsilon}{\epsilon}\left(\underbrace{\nabla\phi_{pol} + \nabla\phi_o}_{\nabla\phi}\right) \tag{12.61}$$

Suppose: fields cancel! $\epsilon = 1$ $\epsilon = \infty$

$$W = \frac{1}{2}\int\int \frac{(\rho_o(\mathbf{r}) + \sigma_{pol}(\mathbf{r}))\,(\rho_o(\mathbf{r}') + \sigma_{pol}(\mathbf{r}'))}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' \tag{12.62}$$

$$\frac{\delta W}{\delta \sigma_{pol}} = 0 \tag{12.63}$$

$$\frac{\delta W}{\delta \sigma_{pol}} = \frac{1}{2}\boldsymbol{\rho}_o^T \cdot \mathbf{G}_o \cdot \boldsymbol{\rho}_o + \boldsymbol{\sigma}_{pol}^T \cdot \mathbf{B}\boldsymbol{\rho}_o + \frac{1}{2}\boldsymbol{\sigma}_{pol}^T \cdot \mathbf{A} \cdot \boldsymbol{\sigma}_{pol} \tag{12.64}$$

$$\frac{\delta W}{\delta \boldsymbol{\sigma}_{pol}} = \mathbf{B}\boldsymbol{\rho}_o + \mathbf{A}\boldsymbol{\sigma}_{pol} = 0 \tag{12.65}$$

$$\sigma_{pol} = \sum_k \sigma_{pol,k} f_k(\mathbf{r}) \qquad\qquad \rho_o = \sum_\ell \rho_{o,\ell}\, g_k(\mathbf{r})$$

$$\boldsymbol{\sigma}_{pol} = -\mathbf{A}^{-1} \cdot \mathbf{B} \cdot \boldsymbol{\rho}_o \tag{12.66}$$

sq. sym.

$$A_{ij} = \int\int \frac{f_i(\mathbf{r}) f_j(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' \tag{12.67}$$

Not sq. or sym.

$$B_{ij} = \int\int \frac{f_i(\mathbf{r}) g_j(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' \tag{12.68}$$

$$\begin{aligned} W =& \frac{1}{2}\boldsymbol{\rho}_o^T \cdot \mathbf{G}_o \cdot \boldsymbol{\rho}_o - \boldsymbol{\rho}^T \cdot \mathbf{B}^T \cdot \mathbf{A}^{-1} \cdot \mathbf{B} \cdot \boldsymbol{\rho}_o + \frac{1}{2}\boldsymbol{\rho}_o^T \cdot \mathbf{B}^T \cdot A^{-1} \cdot \mathbf{B} \cdot \boldsymbol{\rho}_o \\ =& \frac{1}{2}\boldsymbol{\rho}_o^T \cdot \mathbf{G}_o \cdot \boldsymbol{\rho}_o - \frac{1}{2}\boldsymbol{\rho}_o^T \cdot \underbrace{\mathbf{B}^T \cdot \mathbf{A}^{-1} \cdot \mathbf{B} \cdot \boldsymbol{\rho}_o}_{\mathbf{G}_{pol}} \\ =& \frac{1}{2}\boldsymbol{\rho}_o^T \cdot [\mathbf{G}_o + \mathbf{G}_{pol}]\,\boldsymbol{\rho}_o \end{aligned} \tag{12.69}$$

$$\mathbf{G}_{pol} = \mathbf{B}^T \cdot \mathbf{A}^{-1} \cdot \mathbf{B}$$

This is the “Conductor like screening model” COSMO

Chapter 13

Expansions in Orthogonal Functions

The scalar product (or inner product) of two functions (in general complex) over the interval $a \leq x \leq b$ is denoted (f, g) and is defined by

$$(f, g) \equiv \int_a^b f^*(x)g(x)dx$$

For functions of more than one variable,

$$(f, g) \equiv \int_v f^*(\mathbf{r})g(\mathbf{r})dr$$

The scalar product with respect to weighting function $w(x)$ or $w(\mathbf{r})$ is

$$(f, g)_w \equiv \int_a^b f^*(x)g(x)w(x)dx = (f, gw)$$

or

$$(f, g)_w \equiv \int_v f^*(\mathbf{r})g(\mathbf{r})w(\mathbf{r})dr = (f, gw)$$

where the weighting function w is real, nonnegative and integrable over the region involved, and can vanish at only a finite number of points in the region.

The above deinitions of scalar products, both with and without a weighting function, satisfy the basic requirements of a scalr product in any linear vector space, namely:

1. (f, g) is a compex number, and $(f, g)^* = (g, f)$

2. $(f, c_1g_1 + c_2g_2) = c_1(f, g_1) + c_2(f, g_2)$

3. $(f, f) \geq 0$, real, and $(f, f) = 0$ $f = 0$ “almost everywhere”, i.e., $f = 0$ except at a finite number of points in the region.

From these properties other important relations follow. For example

$$(c_1f_1 + c_2f_2, g) = c_1^*(f_1, g) + c_2^*(f_2, g)$$

Proof:

$$\begin{aligned}(c_1f_1 + c_2f_2, g) =& (g, c_1f_1 + c_2f_2)^* && \text{from 1.}\\ =& [c_1(g, f_1) + c_2(g, f_2)]^* && \text{from 2.}\\ =& c_1^*(g, f_1)^* + c_2^*(g, f_2)^* = c_1^*(f_1, g) + c_2^*(f_2, g) && \text{from 1. Q.E.D.}\end{aligned}$$

13.1 Schwarz inequality

An important consequence of the basic properties of a scalar product is the Schwarz inequality:

$$\begin{aligned}|(f,g)|^2 \leq& (f,f)(g,g)\\ &\text{or}\\ |(f,g)| \leq& \|f\|\,\|g\|\end{aligned}$$

where $\|f\| \equiv (f,f)^{\frac{1}{2}}$ is called the norm of f.

Proof of the Schwarz inequality:
$(f+\lambda g, f+\lambda g) \geq 0$ for any complex number λ, and $= 0$ if and only if $f = -\lambda g$, proportional

$$(f,f) + \lambda(f,g) + \lambda^*(g,f) + \lambda^*\lambda(g,g) \geq 0$$

If $(g,g) \neq 0$, choose $\lambda = -\frac{(f,g)^*}{(g,g)}$, so

$$(f,f) - \frac{(f,g)^*}{(g,g)}(f,g) - \frac{(f,g)}{(g,g)}(g,f) + \frac{(f,g)}{(g,g)}\frac{(f,g)^*}{(g,g)}(g,g) \geq 0$$

$$(f,f) = (f,f)^*$$

$$(f,f)(g,g) \geq (f,g)(g,f) = |(f,g)|^2 \tag{13.1}$$

If $(g,g) = 0$, then $g = 0$, so $(f,g) = (f,0) = 0$, and the equality is clearly satisfied.

13.2 Triangle inequality

$$\|f+g\| \leq \|f\| + \|g\| \text{ and } \|f-g\| \geq |\,\|f\| - \|g\|\,|$$

Follow from the basic properties of a scalar product, and the Schwarz inequality.

Proof:

$$\begin{aligned}0 \leq \|f+\lambda g\|^2 =& (f+\lambda g, f+\lambda g)\\ =& (f,f) + \lambda(f,g) + \lambda^*(g,f) + \lambda^*\lambda(g,g)\end{aligned}$$

For $\lambda = 1$,

$$\begin{aligned}\|f+g\|^2 =& (f,f) + (g,g) + (f,g) + (f,g)^* = \|f\|^2 + \|g\|^2 + 2Re(f,g)\\ \leq& \|f\|^2 + \|g\|^2 + 2|(f,g)|, \text{ since } Re\,z \leq |z| \text{ for any complex } z\\ \leq& \|f\|^2 + \|g\|^2 + 2\|f\|\,\|g\|, \text{ from the Schwarz inequality}\\ \leq& (\|f\| + \|g\|)^2\end{aligned}$$

$$\|f+g\| \leq \|f\| + \|g\|$$

For $\lambda = -1$,

$$\begin{aligned}\|f-g\|^2 =&\|f\|^2+\|g\|^2-2Re(f,g)\\ \geq&\|f\|^2+\|g\|^2-2|(f,g)|\\ \geq&\|f\|^2+\|g\|^2-2\|f\|\,\|g\|\\ =&(\|f\|-\|g\|g\|)^2\end{aligned}$$

$$\|f-g\| \geq |\ \|f\|-\|g\|\ |, \text{ Q.E.D.}$$

Definition 1 *f is <u>normalized</u> if and only if $\|f\| = (f,f)^{\frac{1}{2}} = 1$*

Definition 2 *f and g are <u>orthogonal</u> if and only if $(f,g) = 0$*

Definition 3 *The set u_i, $i = 1, 2, \ldots$ is said to be <u>orthonormal</u> if each u_i is normalized and is orthogonal to the other u_i*

Definition 4 *For an orthonormal set u_i, $(u_i, u_j) = \delta_{ij}$*

13.3 Schmidt Orthogonalization Procedure

From any set of <u>linearly independent</u> functions (or vectors) v_i, $i = 1, 2, \ldots$ one can construct the same number of <u>orthonormal</u> functions u_i as follows:

$$\begin{aligned}u_1 =&\frac{v_i}{\|v_1\|}, \text{ normalized}\\ u_2 =&\frac{v_2-(u_1,v_2)u_1}{\|''\|}, \text{ so normalized, at } (u_2,u_1)=0\\ u_3 =&\frac{v_3-(v_3,u_1)u_1-(v_3,u_2)u_2}{\|''\|}, \text{ normalized, at } (u_3.u_1)=0, (u_3,u_2)=0\\ u_i =&\frac{v_1-\sum_{j=1}^{i-1}(v_i,u_j)u_j}{\|''\|}=0, \text{ normalized, at } (u_1,u_k)=0, \quad k<i,\end{aligned}$$

since

$$(u_i,u_k) = \frac{(v_i,u_k)-\sum_{j=1}^{i-1}(v_i,u_j)\overbrace{(u_j,u_k)}^{\delta_{jk}}}{\|\qquad\|} = 0, \quad k<1$$

None of the u_i vanish (and hence they are normalizable) because the v_i are linearly independent. Otherwise the procedure might fail. The procedure is not unique, because the order in which one uses (lables) the original v_i is arbitrary.

$$\begin{aligned}(u_1, v_2-(v_2,u_1)u_1) =&(u_1,v_2)-(v_2,u_1)(u_1,u_1)\\ =&(u_1,v_2)-(u_1,v_2)=0\end{aligned}$$

13.4 Expansions of Functions

Given an enumerably infinite orthonormal set u_i, $i = 1, 2, \ldots$, it is sometimes possible to expand an arbitrary function f (from a particular class of functions) in the infinite series:

$$f(x) = \sum_{i=1}^{\infty} c_i u_i(x) \text{ for some range of } x \text{ (or } \mathbf{r}\text{).}$$

The principal topic of this chapter is the investigation of the nature of such expansions, and the conditions under which such a series converges to the function f, or represents it in some other useful way.

If there is a set of c_i such that the series $\sum_{i=1}^{\infty} c_i u_i(x)$ converges uniformly, and hence defines a continuous function, and that function equals $f(x)$, then the c_i must be related to f by $c_i = (u_i, f)$, since, if $f = \sum_{i=1}^{\infty} c_i u_i$, and the series converges uniformly, so it can be integrated term-by-term,

$$\begin{aligned}\int_a^b u_j^* f dx =& (u_j, f) \\ =& \sum_{i=1}^{\infty} c_i \int_a^b u_j^* u_i dx \\ =& \sum_{i=1}^{\infty} c_i \underbrace{(u_j, u_i)}_{\delta_{ji}} \\ =& c_j\end{aligned}$$

$c_i = (u_i, f)$, called the <u>Fourier coefficient</u> or f with respect to the u_i. If there is a weighting function w,

$$c_i = (u_i, f)_w = \int_a^b u_i^* f w \, dx$$

This expression for the coefficients c_i in a series $\sum_i c_i u_i$ representing f can be arrived at in different mannor. Suppose one wants to approximate f by a finite series $\sum_{i=1}^{n} a_1 u_i$ in the "least squares sense", or "in the mean", by determining the a_i such that

$$M \equiv (f - \sum_{i=1}^{n} a_i u_i, f - \sum_{i=1}^{n} a_i u_i)_w = \int_a^b \left| f - \sum_{i=1}^{n} a_i u_i \right|^2 w \, dx$$

is a minimum. For any choice of the a_i, $M \geq 0$, so

$$\begin{aligned}0 \leq M =& (f, f)_w - \left(f, \sum_{i=1}^{n} a_i u_i \right)_w - \left(\sum_{i=1}^{n} a_i u_i, f \right)_w + \left(\sum_{j=1}^{n} a_i u_i, \sum_{j=1}^{n} a_j u_j \right)_w \\ =& (f, f)_w - \sum_{i=1}^{n} a_i (f, u_i)_w - \sum_{i=1}^{n} a_i^* (u_i, f)_w + \sum_{i=1}^{n} \sum_{j=1}^{n} a_i^* a_j \underbrace{(u_i, u_j)_w}_{\delta_{ij}}\end{aligned}$$

Since $(u_i, u_j)_w = \delta_{ij}$, $(u_i, f)_w = c_i$, and $(f, u_i)_w = (u_i, f)_w^* = c_i^*$,

$$\begin{aligned}0 \leq M =& (f, f)_w - \sum_{i=1}^{n} a_i c_i^* - \sum_{i=1}^{n} a_i^* c_i + \sum_{i=1}^{n} a_i^* a_i \\ =& (f, f)_w + \sum_{i=1}^{n} |a_i - c_i|^2 - \sum_{i=1}^{n} |c_i|^2\end{aligned}$$

Clearly M is a minimum if $a_i = c_i = (u_i, f)_w$, the Fourier coefficient.
The minimum value is:

$$\begin{aligned} M_{min} =& \| f - \sum_{i=1}^{n} c_i u_i \|^2 \\ =& \int_a^b \left| f - \sum_{i=1}^{n} c_i u_i \right|^2 w \, dx \\ =& (f, f)_w - \sum_{i=1}^{n} |c_i|^2 \geq 0 \end{aligned}$$

So

$$(f, f)_w \equiv \int_a^b |f|^2 w \, dx \geq \sum_{i=1}^{n} |c_i|^2$$

Taking the limit as $h \to \infty$:

$$\int_a^b |f|^2 w \, dx \geq \lim_{n \to \infty} \sum_{i=1}^{n} |c_i|^2 = \sum_{i=1}^{\infty} |c_i|^2 \qquad \underline{\text{Bessel's inequality}}$$

Hence, if $\int_a^b |f| w \, dx$ exists, then the series $\sum_{i=1}^{\infty} |c_i|^2$ converges, so $\lim_{h \to \infty} |c_i|^2 = 0$. Therefore, $\lim_{h \to \infty} c_i = 0$.

This remarkable result will be used later in the proof of the convergence of Fourier series.

Definition 5 *The set u_i, $i = 1, 2, \ldots$, is said to be complete with respect to some class of functions if for any function f of the class.*

$$\lim_{n \to \infty} \| f - \sum_{i=1}^{n} c_i u_i \|^2 = 0$$

or equivalently if:

$$\lim_{n \to \infty} \int_a^b \left| f - \sum_{i=1}^{n} c_i u_i \right|^2 w \, dx = 0 \tag{13.2}$$

(Bessel's Inequality becomes an equality) or

$$(f, f)_w = \sum_{c=1}^{\infty} |c_i|^2 \tag{13.3}$$

The last equation is called a completeness relation.

Definition 6 *The completeness relation is a special case of a more general realtion called Parseval's relation:*

If the set u_i is complete, and $'f \quad c_i \equiv (u_i, f)_w, \quad b_i \equiv (u_i, g)_w$, then $(f, g)_w = \sum_{i=1}^{\infty} c_i^* b_i$.

u_1 complete means:

$$\lim_{n \to \infty} \| f - \sum_{i}^{n} c_i u_i \|^2 = 0$$

Proof:

$$\begin{aligned}
|(f,g)_w - \sum_{i=1}^{n} c_i^* b_i| =& |(f,g)_w - \sum_{i=1}^{n}(f,u_i)_w b_i| \\
=& |(f,g)_w - (f, \sum_{i=1}^{n} b_i u_i)_w| \\
=& |(f, g - \sum_{i=1}^{n} b_i u_i)_w| \\
\leq& \|f\| \, \|g - \sum_{i=1}^{n} b_i u_i\|
\end{aligned}$$

from the Schwarz inequality $\quad |(f,g)| \leq \|f\| \, \|g\|$

Hence:

$$\lim_{n\to\infty} |(f,g)_w - \sum_{i=1}^{n} c_i^* b_i| \leq \|f\| \lim_{n\to\infty} \|g - \sum_{i=1}^{n} b_i u_i\| = 0$$

$$\lim_{n\to\infty} \left[(f,g) - \sum_{i=1}^{n} c_i^* b_i \right] = 0$$

because

$$\lim_{n\to\infty} \|g - \sum_{i=1}^{n} b_i u_i\| = 0 \quad \text{since the } u_i \text{ are complete.}$$

Hence $(f,g)_w = \sum_{i=1}^{\infty} c_i^* b_i$ It is important to note that, even if the set of u_i is complete, so that

$$\lim_{n\to\infty} \int_a^b \left| f - \sum_{i=1}^{n} c_i u_i \right|^2 w \, dx = 0 \tag{13.4}$$

it does not necessarily mean that $f = \sum_{i=1}^{\infty} c_i u_i$, even almost everywhere. Sufficient conditions for the latters to be true, in addition to the set u_i being complete, are that the f and u_i be continuous, and the series $f = \sum_{i=1}^{\infty} c_i u_i$ converge uniformly.

Proof:

$$\begin{aligned}
\int_a^b \left| f - \sum_{i=1}^{\infty} c_i u_i \right|^2 w \, dx =& \int_a^b \left[f^* f - f^* \sum_{i=1}^{\infty} c_i u_i - \sum_{i=1}^{\infty} c_i^* u_i^* f + \left(\sum_{i=1}^{\infty} c_i^* u_i^* \right) \left(\sum_{j=1}^{\infty} c_j u_j \right) \right] w \, dx \\
=& (f,f)w - \sum_{i=1}^{\infty} c_i (f, u_i) - \sum_{i=1}^{\infty} c_i^* (u_i, f) + \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} c_i^* c_j (u_i, u_j)
\end{aligned}$$

because $\sum_{i=1}^{\infty} c_i u_i$ converges uniformly, so it is a continuous function, and the series can be integrated term-by-term. Since $c_i = (u_i, f)$, $(u_i, u_j) = J_{ij}$,

$$\int_b^a |f - \sum_{i=1}^{\infty} c_i u_i|^2 w \, dx = (f,f)_w - \sum_{i=1}^{\infty} |c_i|^2$$

if the system converges uniformly.

But also we know that

$$\lim_{n\to\infty}\int_a^b \left|f-\sum_{i=1}^{\infty} c_i u_i\right|^2 w\,dx = (f,f)_w - \sum_{i=1}^{\infty}|c_i|^2$$

$$f \equiv \sum_{i=1}^{\infty} c_i u_i$$

if the series converges uniformly and lim can then be moved inside the integration.

Hence, if the series converges uniformly,

$$\begin{aligned}\int_a^b \left|f-\sum_{i=1}^{\infty} c_i u_i\right|^2 w\,dx = &\lim_{n\to\infty}\int_a^b \left|f-\sum_{i=1}^{n} c_i u_i\right|^2 w\,dx \\ =&0 \qquad \text{if the set is complete}\end{aligned}$$

But if the series converges uniformly, it is a continuous function. If f is also continuous, $f = \sum_{i=1}^{\infty} c_i u_i$ is continuous, and the integral can vanish only if $f - \sum_{i=1}^{\infty} c_i u_i = 0$, or $f = \sum_{i=1}^{\infty} c_i u_i$, $a \le x \le b$ Q.E.D.

Theorem 1 *(Dettman p.335) A uniformly convergent sequence of continuous functions converges to a continuous function*

Definition 7 *The set of vectors (functions) u_i, $i = 1, 2, \ldots$, is said to be closed if any function orthogonal to all the u_i must have zero norm, and hence is zero almost everywhere. That is, if:*

$$(u_i, f) = 0 \qquad \text{, then} \qquad \|f\| = (f,f)_w^{\frac{1}{2}} = 0$$

Theorem 2 *If a set of u_i is complete, then it is closed.*

Proof: Since the set is complete,

$$\lim_{n\to\infty}\int_a^b \left|f-\sum_{i=1}^{n}(u_i,f)u_i\right|^2 w\,dx = 0$$

So any function f orthogonal to all the u_i satisfies:

$$\begin{aligned}\lim_{n\to\infty}\int_a^b |f-0|^2 w\,dx =&0 \\ =&\int_a^b |f|^2 w\,dx \\ =&\|f\|^2\end{aligned}$$

$$\|f\| = 0$$

The converse is also true for square-integrable functions, but the proof requires some preliminary discussion.

Definition 8 *Definition: An infinite sequence q_n, $n = 1, 2, \ldots$ of vecotrs in a linear vector space (such as a sequence of square-integrable functions) is said to form a Cauchy sequence if, given any $\epsilon > 0$, there is an integer N such that $\|g_n - g_m\| < \epsilon$ if $n, m > N$.*

Definition 9 *A linear vector space is said to be complete if every Cauchy sequence of vectors in the space has a limit vector in the space, such that $\lim_{n\to\infty} \|g - g_n\| = 0$, where g is called the limit of the sequence g_n.*

Definition 10 *A Hilbert space is an infinitely-dimensional complex complete linear vector spece with a scaler product.*

Theorem 3 *(Riesz-Fischer theorem) Every Cauchy sequence of square-integrable functions has a limit, which is a square-integrable function.*

Hence the space of square-integrable functions is a Hilbert space. We are now ready to prove the following:

Theorem 4 *If the set of orthonormal functions u_i, $i = 1, 2, \ldots$ is closed, then it is complete.*

Proof: Let f be any square-integrable function, and $g_n \equiv f - \sum_{i=1}^{n} c_i u_i$, where $c_i = (u_i, f)$. Then:

$$\begin{aligned}
(u_k, g_n) =& (u_k, f - \sum_{i=1}^{n} c_i u_i) \\
=& (u_k, f) - \sum_{i=1}^{n} c_i (u_k, u_i) \\
=& (u_k, f) - \sum_{i=1}^{n} c_i \delta_{ki}, \qquad \text{since } (n_k, u_i) = J_{ki} \\
=& 0 \qquad \text{if} \qquad k \le n
\end{aligned}$$

Next consider:

$$\begin{aligned}
\|g_n - g_m\|^2 =& \|f - \sum_{i=1}^{n} c_i u_i - f + \sum_{i=1}^{m} c_i u_i\|^2 \\
=& \|\sum_{i=n+1}^{m} c_i u_i\|^2, \quad \text{where } m > n \\
=& \left(\sum_{i=n+1}^{m} c_i u_i, \sum_{j=n+1}^{m} c_j u_j \right) \\
=& \sum_{i=n+1}^{m} \sum_{j=n+1}^{m} c_i^* c_j \underbrace{(u_i, u_j)}_{\delta_{ij}} \\
=& \sum_{i=n+1}^{m} |c_i|^2
\end{aligned}$$

But from Bessel's inequality $(f, f) \ge \sum_{i=1}^{\infty} |c_i|^2$, it follows that the series converges, so for any $\epsilon > 0$ there is an integer N such that $\sum_{i=n+1}^{m} |c_i|^2 < \epsilon$ for $m > n > N$. Hence the g_n from a Cauchy sequence of square-integrable functions, and hence there is a square-integrable function g such that

$$\lim_{n\to\infty} \|g - g_n\| = 0 \qquad \text{(Riesz-Fischer)}$$

Therefore:

$$\begin{aligned}\lim_{n\to\infty}\|g_n\| &= \lim_{n\to\infty}\|g_n - g + g\| \\ &\leq \lim_{n\to\infty}\{\|g_n - g\| + \|g\|\} \\ &= \|g\|\end{aligned}$$

Furthermore, for given k and $n > k$,

$$\begin{aligned}|(u_k, g)| =& |(u_k, g - g_n)| \quad \text{since} \quad (u_k, g_n) = 0 \text{ for } n > k \\ \leq& \|u_k\|\,\|g - g_n\| \\ =& \|g - g_n\| \quad \text{from the Schwarz inequality, and } \|u_k\| = 1\end{aligned}$$

Hence:

$$\lim_{n\to\infty}|(u_k, g)| \leq \lim_{n\to\infty}\|g - g_n\| = 0$$

so $|(u_k, g)| = 0$ and $(u_k, g) = 0$

So the limit function g is orthogonal to all the u_k (hence closed). Hence, if the set of u_k is closed, then $\|g\| = 0$. But then

$$\lim_{n\to\infty}\|g_n\| = \|g\| = 0$$

or

$$\lim_{n\to\infty}\int_a^b \left|f - \sum_{i=1}^n c_i u_i\right|^2 w\,dx = 0 \quad \text{(means } u_i \text{ is complete)}$$

and we have proved that the set of orthonormal u_i is complete if it is closed.

Definition 11 *A real function $f(x)$ is piecewise continuous (or sectionally continuous) on an interval $a \leq x \leq b$ if the interval can be subdivided into a finite number of intervals in each of which $f(x)$ is continuous and approaches finite limits at the end.*

If $f(x)$ is a complex function of the real variable x, it is piecewise continuous and both its real and imaginary parts are piecewise continuous.

Definition 12 *A function $f(x)$ is piecewise smooth if both $f(x)$ and its derivative $f'(x)$ are piecewise continuous.*

Example: $f(x)$ is continuous, and $f'(x)$ is piecewise continuous on $a \leq x \leq b$ so $f(x)$ is piecewise smooth.
Example: both $f(x)$ and $f'(x)$ are piecewise continuous, so $f(x)$ is piecewise smooth.

Definition 13

$$f(x+) \equiv \lim_{0<\epsilon\to 0} f(x+\epsilon)$$

Definition 14

$$f(x-) \equiv \lim_{0<\epsilon\to 0} f(x-\epsilon)$$

Definition 15

$$f'(x) \equiv \lim_{\Delta x\to 0}\frac{f(x+\Delta x) - f(x)}{\Delta x}$$

which means that, given any $\epsilon > 0$, there is a $J > 0$ such that $f'(x)$ exists so that

$$\left|f'(x) - \frac{f(x+\Delta x) - f(x)}{\Delta x}\right| < \epsilon \textit{ if } |\Delta x| < \delta$$

So in the definition $f'(x) \equiv \lim_{\Delta x \to 0} \frac{f(x+\Delta x)-f(x)}{\Delta x}$, the limit must exist and be independent of whether $\Delta x \to 0$ through positive or negative values.

Definition 16 *The right-hand derivative of $f(x)$ at x is*

$$f'_R(x) \equiv \lim_{0<\Delta x \to 0} \frac{f(x+\Delta x)-f(x+)}{\Delta x}$$

Definition 17 *The left-hand derivative is*

$$f'_R(x) \equiv \lim_{0<\Delta x \to 0} \frac{f(x-)-(x-\Delta x)}{\Delta x}$$

At a point at which $f'(x)$ exists, $f'_R(x) = f'_L(x) = f'(x)$ If $f(x)$ is piecewise smooth, then $f'_R(x) = f'(x+)$ and $f'_L(x) = f'(x-)$, and these exist at each point.

13.5 Fourier Series

Reference: Churchill, Fourier Series and Boundary Value Problems

The set of functions $\{\frac{1}{\sqrt{2\pi}}, \frac{1}{\sqrt{\pi}}\cos nx, \frac{1}{\sqrt{\pi}}\sin nx\}$, $n = 1, 2, \ldots$, is orthonormal over any interval of length 2π. Consider the interval $-\pi \le x \le \pi$. The series best representing $f(x)$ in the least-squares sense has coefficients $c_n = (u_m f)$, so the series is

$$\begin{aligned}
&\left(\frac{1}{\sqrt{2\pi}}, f\right)\frac{1}{\sqrt{2\pi}} + \sum_{n=1}^{\infty}\left[\left(\frac{1}{\sqrt{\pi}}\cos nx, f\right)\frac{1}{\sqrt{\pi}}\cos nx + \left(\frac{1}{\sqrt{\pi}}\sin nx, f\right)\frac{1}{\sqrt{\pi}}\sin nx\right] \\
&= \frac{1}{\sqrt{2\pi}}(1, f) + \sum_{n=1}^{\infty}\left[\left(\frac{1}{\sqrt{\pi}}\cos nx, f\right)\cos nx + \frac{1}{\pi}(\sin nx, f)\sin nx\right] \\
&= \frac{A_o}{2} + \sum_{n=1}^{\infty}[A_n \cos nx + B_n \sin nx]
\end{aligned}$$

where

$$\begin{aligned}
A_n &= \frac{1}{\pi}(\cos nx, f) = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos nx\, dx, n = 0, 1, 2, \ldots \\
B_n &= \frac{1}{\pi}(\sin nx, f) = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin nx\, dx
\end{aligned}$$

This Trignometric series with the coefficients A_n and B_n is called the Fourier series for $f(x)$ over $-\pi \le x \le \pi$

13.6 Convergence Theorem for Fourier Series

If $f(x)$ is piecewise continuous and periodic with period 2π for all x, and if, at points of discontinuity $f(x)$ is defined by:

$$f(x) \equiv \frac{1}{2}[f(x+) + f(x-)] \tag{13.5}$$

then

$$f(x) = \frac{A_o}{2}\sum_{n=1}^{\infty}[A_n \cos nx + B_n \sin nx] \tag{13.6}$$

where

$$A_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos nx\,dx \qquad\qquad B_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin nx\,dx$$

at all points where $f(x)$ has finite right and left derivatives. This includes all points if $f(x)$ is piecewise smooth. If $f(x)$ is not periodic, the expansion is valid for $-\pi \leq x \leq \pi$, with the series converging to $\frac{1}{2}[f(\pi-)+f(-\pi+)]$ at $x = \pm\pi$.

Lemma 1 *If $\int_0^{\pi} |g(x)|^2 dx$ exists, then*

$$\lim_{n\to\infty}\int_0^{\pi} g(x)\cos Nx\,dx = 0 \quad \textit{and} \quad \lim_{N\to R}\int_0^{\pi} g(x)\sin Nx dx = 0$$

Proof: The functions $\sqrt{\frac{2}{\pi}}\sin Nx$, $N = 1, 2, \ldots$ are orthonormal over $0 \leq x \leq \pi$. Hence Bassel's inequality gives:

$$\int_0^{\pi} |g(x)|^2 dx \geq \sum_{N=1}^{\infty}\left|\int_0^{\pi}\sqrt{\frac{2}{\pi}}\sin Nx g(x)dx\right|^2$$

so the series converges.

Hence

$$\lim_{n\to\infty}\int_0^{\pi}\sin Nx g(x)\,dx = 0$$

Similarily, the set $\{\frac{1}{\sqrt{\pi}}, \sqrt{\frac{2}{\pi}}\cos Nx\}$ is orthonormal over $0 \leq x \leq \pi$, so

$$\lim_{n\to\infty}\int_0^{\pi}\cos Nx g(x)\,dx = 0 \qquad \text{Q.E.D.}$$

$$A_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos nx\,dx \qquad\qquad B_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin nx\,dx$$

We are now ready to prove the convergence Th. for Fourier series. The partial sum of the Fourier series is

$$\begin{aligned}
S_N(x) =& \frac{1}{2}A_o + \sum_{n=1}^{N}[A_n\cos nx + B_n\sin nx] \\
=& \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x')dx' + \sum_{n=1}^{N}\left\{\left[\frac{1}{\pi}\int_{-\pi}^{\pi} f(x')\cos nx'dx'\right]\cos nx + \left[\frac{1}{\pi}\int_{-\pi}^{\pi} f(x')\sin nx'dx'\right] sinnx\right\} \\
=& \frac{1}{2\pi}\int_{-\pi}^{\pi} dx' f(x')\left\{1 + 2\sum_{n=1}^{N}[\cos nx'\cos nx + sinnx'\sin nx]\right\} \\
=& \frac{1}{2\pi}\int_{-\pi}^{\pi} dx' f(x')\left\{1 + 2\sum_{n=1}^{N}\cos ny\right\}
\end{aligned}$$

Change the variable of integration to $y = x' - x$, so $dy = dx'$, and

$$S_N(x) = \frac{1}{2\pi}\int_{-\pi-x}^{\pi-x} dy\, f(y+x)\left\{1 + 2\sum_{n=1}^{N}\cos ny\right\}$$

Since the integrand is periodic with period 2π, $\int_{-\pi-x}^{\pi-x} = \int_{-\pi}^{\pi}$. Also, the series can be summed as follows:

$$\begin{aligned} F_N =& 1 + 2\sum_{n=1}^{N} \cos ny \\ =& 1 + 2\sum_{n=1}^{N} \frac{(e^{iny} + e^{-iny})}{2} \\ =& \sum_{n=-N}^{N} e^{iny} \end{aligned} \tag{13.7}$$

so

$$e^{iny} F_N - F_N = e^{i(N+1)y} - e^{-iNy}$$

$$\begin{aligned} F_N =& \frac{e^{i(N+1)y} - e^{-iNy}}{e^{iy} - 1} \\ =& \frac{e^{i\frac{y}{2}}(e^{i(N+\frac{1}{2})y} - e^{-i(N+\frac{1}{2})y})}{e^{i\frac{y}{2}}(e^{i\frac{y}{2}} - e^{-i\frac{y}{2}})} \\ =& \frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} \end{aligned} \tag{13.8}$$

Hence

$$1 + 2\sum_{n=1}^{N} \cos ny = \frac{sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} \tag{13.9}$$

Therefore also

$$\begin{aligned} \frac{1}{\pi}\int_0^{\pi} \frac{sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} dy =& \frac{1}{\pi}\int_0^{\pi} \left[1 + 2\sum_{n=1}^{N} \cos ny\right] dy \\ =& \frac{1}{\pi}\left[y + 2\sum_{n=1}^{N} \frac{\sin ny}{n}\right]_0^{\pi} \\ =& 1 \end{aligned}$$

so

$$\frac{1}{\pi}\int_0^{\pi} \frac{sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} dy = 1 \tag{13.10}$$

Using the Eq. (13.9) above in the last expression for $S_N(x)$ gives

$$\begin{aligned} S_N(x) =& \frac{1}{2\pi}\int_{-\pi}^{\pi} dy\, f(y+x) \frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} \\ =& \frac{1}{2\pi}\int_0^{\pi} dy\, f(y+x) \frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} dy + \frac{1}{2\pi}\int_{-\pi}^{0} dy' f(y'+x) \frac{\sin(N+\frac{1}{2})y'}{\sin\frac{y'}{2}} \end{aligned}$$

Replacing y' by $-y$ in the second integral,

$$\begin{aligned}S_N(x) =&\frac{1}{2\pi}\int_0^\pi dy\, f(y+x)\frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}}dy + \frac{1}{2\pi}\int_0^\pi dy\, f(-y+x)\frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}} \\ =&\frac{1}{2\pi}\int_0^\pi [f(x+y)+f(x-y)]\frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}}dy \qquad (13.11)\end{aligned}$$

From Eq. (13.10) it follows that

$$\frac{1}{2}[f(x+)+f(x-)] = \frac{1}{2\pi}\int_0^\pi [f(x+)+f(x-)]\frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}}dy \qquad (13.12)$$

Subtracting Eq. (13.12) from Eq. (13.11) we obtain:

$$\begin{aligned}S_N(X) - \frac{1}{2}[f(x+)+f(x-)] =&\frac{1}{2\pi}\int_0^\pi [f(x+y)-f(x+)+f(x-y)-f(x-)]\frac{\sin(N+\frac{1}{2})y}{\sin\frac{y}{2}}dy \\ =&\frac{1}{\pi}\int_0^\pi \phi(y)\sin(N+\frac{1}{2})y\,dy \qquad (13.13)\end{aligned}$$

where

$$\begin{aligned}\phi(y) \equiv&\frac{[f(x+y)-f(x+)+f(x-y)-f(x-)]}{2\sin\frac{y}{2}} \\ =&\left\{\frac{[f(x+y)-f(x+)]}{y} - \frac{[f(x-)-f(x-y)]}{y}\right\}\frac{\left(\frac{y}{2}\right)}{\sin\frac{y}{2}} \qquad (13.14)\end{aligned}$$

From Eq. (13.13),

$$\begin{aligned}&\lim_{N\to\infty}\left\{S_N(x) - \frac{1}{2}[f(x+)+f(x-)]\right\} \\ &= \lim_{N\to\infty}\frac{1}{\pi}\int_0^\pi \phi(y)\sin(N+\frac{1}{2})y\,dy \\ &= \lim_{N\to\infty}\frac{1}{\pi}\int_0^\pi \phi(y)\left[\sin Ny\cos\frac{1}{2}y + \cos Ny\sin\frac{1}{2}y\right]dy \\ &= \lim_{N\to\infty}\frac{1}{\pi}\int_0^\pi \left[\phi(y)\cos\frac{1}{2}y\right]\sin Ny dy + \lim_{N\to\infty}\frac{1}{\pi}\int_0^\pi \left[\phi(y)\sin\frac{1}{2}y\right]\cos Ny\,dy \\ &=0 \qquad \text{from the lemma} \qquad (13.15)\end{aligned}$$

if $\phi(y)\cos\frac{1}{2}y$ and $\phi(y)\sin\frac{1}{2}y$ are square integrable over $0 \le y \le \pi$, which is the case if $\phi(y)$ is piecewise continuous for $0 \le y \le \pi$. From the first of expressions Eq. (13.14) for $\phi(y)$ it is apparent that $\phi(y)$ is piecewise continuous on $0 \le y \le \pi$ except possibly at $y = 0$ where $\sin\frac{y}{2}$ vanishes. But from the second expression Eq. (13.14),

$$\begin{aligned}\lim_{0<y\to 0}\phi(y) =& \lim_{0<y\to 0}\left\{\frac{[f(x+y)-f(x+)]}{y} - \frac{[f(x-)-f(x-y)]}{y}\right\}\frac{(\frac{y}{2})}{\sin(\frac{y}{2})} \\ =&f'_R(x) - f'_L(x) \qquad (13.16)\end{aligned}$$

So, at points x for which $f'_R(x)$ and $f'_L(x)$ exist,

$$\begin{aligned}\frac{1}{2}[f(x+)+f(x-)] &= \lim_{N\to\infty} S_N(x) \\ &= \frac{1}{2}A_o + \sum_{n=1}^{\infty}[A_n \cos nx + B_n \sin nx]\end{aligned} \tag{13.17}$$

This completes the proof of the convergence theorem.

$$f(x) \equiv \frac{1}{2}[f(x+)+f(x-)] = \frac{A_o}{2} + \sum_{n=1}^{\infty}\sum_{n=1}^{\infty}[A_n \cos nx + B_n \sin nx]$$

if $f(x)$ is piecewise continuous and periodic (period 2π)

13.7 Fourier series for different intervals

If $g(t)$ is piecewise smooth and periofic with period 2π, it has the Fourier series:

$$g(t) = \frac{1}{2}A_o + \sum_{n=1}^{\infty}[A_n \cos nt + B_n \sin nt] \tag{13.18}$$

where

$$A_n = \frac{1}{\pi}\int_{-\pi}^{\pi} g(t)\cos nt\, dt \qquad B_n = \frac{1}{\pi}\int_{-\pi}^{\pi} g(t)\sin nt\, dt$$

The function $f(x) \equiv g(\frac{\pi}{L}x)$ is piecewise smooth and periodic with period $2L$. Replacing t by $\frac{\pi x}{L}$ in the Fourier series for $g(t)$, we obtain

$$f(x) = \frac{1}{2}A_o + \sum +n = 1^{\infty}\left[A_n \cos\frac{n\pi x}{L} + B_n \sin\frac{n\pi x}{L}\right] \tag{13.19}$$

where

$$\begin{aligned}A_n &= \frac{1}{\pi}\int_{-L}^{L} g\left(\frac{\pi x}{L}\right)\left(\cos\frac{n\pi x}{L}\right)\frac{\pi}{L}dx \\ &= \frac{1}{\pi}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx\end{aligned} \tag{13.20}$$

and

$$\begin{aligned}B_n &= \frac{1}{\pi}\int_{-L}^{L} g\left(\frac{\pi x}{L}\right)\left(\sin\frac{n\pi x}{L}\right)\frac{\pi}{L}dx \\ &= \frac{1}{\pi}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx\end{aligned} \tag{13.21}$$

For a piecewise smooth function $f(x)$, which is periodic with period $2L$, this Fourier series converges to $f(x) \equiv \frac{1}{2}[f(x-)+f(x+)]$ at all x.

A piecewise smooth function $f(x)$ which is not periodic in x can be expanded in a Fourier series in the form of Eqn 1 above, and the series will converge to $f(x) \equiv \frac{1}{2}[f(x-) + f(x+)]$ at all points on any open interval of length $2L$, say $x_o - L \leq x \leq x_o + L$, if the coefficients are determined by:

$$A_n = \frac{1}{L}\int_{x_o-L}^{x_o+L} f(x)\cos\frac{n\pi x}{L}dx \qquad B_n = \frac{1}{L}\int_{x_o-L}^{x_o+L} f(x)\sin\frac{n\pi x}{L}dx \tag{13.22}$$

This is because one can define a function $F(x)$ which is periofic with period $2L$ and which equals $f(x)$ for $x_o - L < x < x_o + L$. $F(x)$ has a Fourier series Eq. (13.19) which equals $f(x)$ for $x_o - L < x < x_o + L$. Since $F(x)$ is periodic with period $2L$, the integrals in A_n and B_n can be taken over any interval of length $2L$, and in particular for $x_o - L < x < x_o + L$, where $F(x) = f(x)$, giving the expressions (13.22). At $x = x_o - L$ and $x = x_o + L$, the series converges to $\frac{1}{2}[f(x_o - L+) + f(x_o + L-)]$.

In particular, for the interval $-L \leq x \leq L$, a piecewise smooth $f(x)$ can be expanded as:

$$f(x) = \frac{1}{2}A_o + \sum_{n=1}^{\infty}\left[A_n\cos\frac{n\pi x}{L} + B_n\sin\frac{n\pi x}{L}\right], \qquad (-L \leq x \leq L) \tag{13.23}$$

where

$$A_n = \frac{1}{\pi}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx \qquad B_n = \frac{1}{\pi}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx$$

If $f(x)$ is an even function, all the $B_n = 0$, and if it is an off function, all the $A_n = 0$. A function which is piecewise smooth for $0 \leq x \leq L$ can be expanded in a Fourier sine series.

$$\begin{aligned} f(x) \equiv& \frac{1}{2}[f(x-) + f(x+)] \\ =& \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{L} \end{aligned} \tag{13.24}$$

where

$$B_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx \tag{13.25}$$

and where the series vanishes at $x = 0$ and $x = L$, or the function can be expanded in a Fourier cosine series

$$f(x) = \frac{1}{2}A_o + \sum_{n=1}^{\infty} A_n\cos\frac{n\pi x}{L} \tag{13.26}$$

where

$$A_n = \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}dx \tag{13.27}$$

and the series converge to $\frac{1}{2}[f(x-) + f(x+)]$ for $0 \leq x \leq L$, to $f(0+)$ for $x = 0$, and to $f(L-)$ at $x = L$.

These results follow from the fact that a piecewise smooth function defined on $0 \leq x \leq L$ can have its definition extended to $-L \leq x \leq L$ in such a way that it is either an odd or an even function of x.

13.8 Complex Form of the Fourier Series

Suppose that $f(x)$ is either a real or complex function which is piecewise smooth on $x_o - L \le x \le x_o + L$. The Fourier series for $f(x)$, valid on that interval, can be written:

$$\begin{aligned}
f(x) =& \frac{1}{2}A_o + \sum_{n=1}^{\infty}\left[A_n \cos\frac{n\pi x}{L} + B_n \sin\frac{n\pi x}{L}\right] \\
=& \frac{1}{2}A_o + \sum_{n=1}^{\infty}\left[A_n\left(\frac{e^{\frac{in\pi x}{L}} + e^{-\frac{in\pi x}{L}}}{2}\right) + B_n\left(\frac{e^{\frac{in\pi x}{L}} - e^{-\frac{in\pi x}{L}}}{2}\right)\right] \\
=& \frac{1}{2}A_o + \sum_{n=1}^{\infty}\left[\frac{1}{2}(A_n - iB_n)e^{\frac{in\pi x}{L}} + \frac{1}{2}(A_n + iB_n)e^{-\frac{in\pi x}{L}}\right]
\end{aligned} \tag{13.28}$$

Let

$$c_n \equiv \frac{1}{2}(A_n - iB_n) = \frac{1}{2L}\int_{x_o-L}^{x_o+L}\left(\cos\frac{n\pi x}{L} - c\sin\frac{n\pi x}{L}\right)f(x)dx$$

$$c_n = \frac{1}{2L}\int_{x_o-L}^{x_o+L} f(x)e^{-\frac{in\pi x}{L}}dx \tag{13.29}$$

Then

$$\frac{1}{2}A_o = \frac{1}{2L}\int_{x_o-L}^{x_o+L} f(x)dx = c_o \tag{13.30}$$

and

$$\begin{aligned}
\frac{1}{2}(A_n + iB_n) =& \frac{1}{2L}\int_{x_o-L}^{x_o+L} f(x)\left[\cos\frac{n\pi x}{L} + i\sin\frac{n\pi x}{L}\right]dx \\
=& \frac{1}{2L}\int_{x_o-L}^{x_o+L} f(x)e^{\frac{in\pi x}{L}}dx \\
=& C_{-n}
\end{aligned} \tag{13.31}$$

Hence

$$f(x) = c_o + \sum_{n=1}^{\infty}\left[c_n e^{\frac{in\pi x}{L}} + c_{-n}e^{-\frac{in\pi x}{L}}\right] \tag{13.32}$$

or

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{in\pi x}{L}} \qquad\qquad x_o - L \le x \le x_o + L$$

This is called the complex form of the Fourier series for $f(x)$, whether or not $f(x)$ itself is complex. It converges to

$$\frac{1}{2}[f(x-) + f(x+)] \quad \text{for} \quad x_o - L < x < x_o - L$$

At $x = x_o - L$ and $x = x_o + L$, it converges to $\frac{1}{2}[f(x_o - L+) + f(x_o + L-)]$.

13.9 Uniform Convergence of Fourier Series

$$f(x) = \frac{A_o}{2} + \sum_{n=1}^{\infty}[A_n \cos nx + B_n \sin nx] \tag{13.33}$$

$$\begin{aligned}(|A| + |B|)^2 =& |A|^2 + |B|^2 + 2|A|\,|B| \\ (|A| - |B|)^2 =& |A|^2 + |B|^2 - 2|A|\,|B| \\ (|A| + |B|)^2 + (|A| - |B|)^2 =& 2(|A|^2 + |B|^2 \geq (|A| + |B|)^2\end{aligned}$$

hence $|A| + |B| \leq \sqrt{2}(|A|^2 + |B|^2)^{\frac{1}{2}}$

$$\begin{aligned}|A_n \cos nx + B_n \sin nx| \leq& |A_n \cos nx| + |B_n \sin nx| \\ \leq& |A_n| + |B_n| \\ \leq& [|A_n|^2 + |B_n|^2]^{\frac{1}{2}} \\ =& \sqrt{2}[A_n^2 + B_n^2]^{\frac{1}{2}}\end{aligned}$$

taking $f(x)$ to be real, so the A_n and B_n are real. Hence the Fourier series for $f(x)$ converges absolutely and uniformly if the series $\sum_{n=1}^{N}[A_n^2 + B_n^2]^{\frac{1}{2}}$ converges.

Let

$$\begin{aligned}S_N \equiv& \sum_{n=1}^{N}[A_n^2 + B_n^2]^{\frac{1}{2}} \\ =& \sum_{n=1}^{N}\frac{1}{n}[n^2(A_n^2 + B_n^2)]^{\frac{1}{2}} \\ =& \sum_{n=1}^{N}\underbrace{\left[\frac{1}{n^2}\right]^{\frac{1}{2}}}_{|c_n|}\underbrace{[n^2(A_n^2 + B_n^2)]^{\frac{1}{2}}}_{|D_n|} \\ \leq& \left[\sum_{n=1}^{N}\frac{1}{n^2}\right]\left[\sum_{n=1}^{N}n^2(A_n^2 + B_n^2)\right]^{\frac{1}{2}}\end{aligned}$$

$$|(c, D)| \leq \|c\|\,\|D\|$$

from the Schwarz inequality in a vector space in which vectors are N-Tuples of real numbers, such as $c \equiv (c_1, c_2 \ldots c_N)$, $d \equiv (d_1, d_2 \ldots d_N$, and the scalar product is defined by $(c, d) \equiv \sum_{n=1}^{N} c_n d_n$. The Schwarz inequality is $|(c, d)| \leq (c, c)^{\frac{1}{2}}(d, d)^{\frac{1}{2}}$, or

$$\sum_{n=1}^{N} c_n d_n \leq \left[\sum_{n=1}^{N} c_n^2 \sum_{n=1}^{N} d_n^2\right]^{\frac{1}{2}} \tag{13.34}$$

With the choice

$$c_n = \frac{1}{n} \qquad d_n = [n^2(A_n^2 + B_n^2)]^{\frac{1}{2}} = n(A_n^2 + B_n^2)^{\frac{1}{2}} \tag{13.35}$$

$$\sum_{n=1}^{N}(A_n^2+B_n^2)^{\frac{1}{2}} \leq \left[\sum_{n=1}^{N}\frac{1}{n^2}\sum_{n=1}^{N}n^2(A_n^2+B_n^2)\right]^{\frac{1}{2}} \tag{13.36}$$

If, for $-\pi \leq x \leq \pi$, $f(x)$ is continuous, $f'(x)$ is piecewise continuous, and $f(-\pi) = f(\pi)$, then the series $\sum_{n=1}^{\infty} n^2(A_n^2 + B_n^2)$ converges, as shown in problem (9). Since the series $\sum_{n=1}^{\infty} \frac{1}{n^2}$ also converges, it follows that $\sum_{n=1}^{\infty}(A_n^2 + B_n^2)^{\frac{1}{2}}$ converges, so the Fourier series for $f(x)$ converges uniformly and absolutely.

$$\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}$$
$$\sum_{n=1}^{\infty}\frac{1}{n^p} = \zeta(p) \quad \text{(Reimann Zeta)}$$

Hence we have proven:

Theorem 5 *If $f(x)$ is continuous and if it is only piecewise continuous and $f'(x)$ is piecewise continuous for $-\pi \leq x \leq \pi$, and $f(-\pi) = f(\pi)$, then the Fourier series for $f(x)$ converges uniformly and absolutely on $-\pi \leq x \leq \pi$ (or any interval that is continuous).*

It can be shown, by a more complicated proof, that the Fourier series for a piecewise smooth function converges uniformly and absolutely in any closed subinterval in which the function is continuous. Piecewise smooth $\equiv$ $f(x)$, $f'(x)$ are piecewise continuous.

13.10 Differentiation of Fourier Series

If $f(x)$ is periodic and continuous, and if $f'(x)$ and $f''(x)$ are piecewise continuous, then the term-by-term derivative of the Fourier series for $f(x)$ equals $f'(x)$ except at points where $f'(x)$ is discontinuous.

Under these conditions both $f(x)$ and $f'(x)$ have convergent Fourier series, and the term-by-term derivation of the series for $f(x)$ equals the series for $f'(x)$. Details are worked out in problem (12.)

13.11 Integration of Fourier Series

If $f(x)$ is piecewise continuous for $-L \leq x \leq L$, then, whether or not the Fourier series $\frac{A_o}{2} + \sum_{n=1}^{\infty}\left[A_n \cos\frac{n\pi x}{L} + B_n \sin\frac{n\pi x}{L}\right]$ corresponding to $f(x)$ converges, the term-by-term integral of the series from $-L$ to $x \leq L$ equals $\int_{-L}^{x} f(x)dx$.

Proof:

$$F(x) \equiv \int_{-L}^{x} f(x)dx - \frac{1}{2}A_o x$$

is a continuous function, with derivative $F'(x) = f(x) - \frac{1}{2}A_o$ which is piecewise continuous on $-L \leq x \leq L$ for $f(x)$ piecewise continuous on $-L \leq x \leq L$

Show $F(x)$ periodic.

Also $F(-L) = \frac{1}{2}A_o L$, and

$$\begin{aligned} F(L) =& \int_{-L}^{L} f(x)dx - \frac{1}{2}A_o L \\ =& LA_o - \frac{1}{2}A_o L \\ =& \frac{1}{2}A_o L = F(-L) \end{aligned}$$

Hence $F(x)$ has a Fourier series

$$F(x) = \frac{a_o}{2} + \sum_{n=1}^{\infty}\left[a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right] \tag{13.37}$$

which converges to $f(x)$ for all points on $-L \le x \le L$. At $x = L$,

$$\begin{aligned} F(L) =& \frac{1}{2}A_o L \\ =& \frac{a_o}{2} + \sum_{n=1}^{\infty}\left[a_n \underbrace{\cos n\pi}_{(-1)^n} + b_n \underbrace{\sin n\pi}_{0}\right] \\ =& \frac{a_o}{2} + \sum_{n=1}^{\infty} a_n(-1)^n \end{aligned}$$

Hence

$$\frac{a_o}{2} = \frac{1}{2}A_o L - \sum_{n=1}^{\infty} a_n(-1)^n \tag{13.38}$$

Also, for $n > 0$

$$\begin{aligned} a_n =& \frac{1}{L}\int_{-L}^{L} F(x)\cos\frac{n\pi x}{L}dx \\ =& \frac{1}{L}\left\{\left[\frac{F(x)\sin\frac{n\pi x}{L}}{\frac{n\pi}{L}}\right]_{-L}^{L} - \int_{-L}^{L}\frac{F'(x)\sin\frac{n\pi x}{L}}{\frac{n\pi}{L}}dx\right\} \\ =& -\frac{1}{n\pi}\int_{-L}^{L} F'(x)\sin\frac{n\pi x}{L}dx \\ =& -\frac{1}{n\pi}\int_{-L}^{L}\left[f(x) - \frac{1}{2}A_o\right]\sin\frac{n\pi x}{L}dx \\ =& -\frac{L}{n\pi}\frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx \\ =& -\frac{L}{n\pi}B_n \qquad \text{for } n > 0 \end{aligned}$$

And

$$\begin{aligned}
b_n =& \frac{1}{L}\int_{-L}^{L} F(x)\sin\frac{n\pi x}{L}dx \\
=& \frac{1}{L}\left\{\left[F(x)\frac{-\cos\frac{n\pi x}{L}}{\frac{n\pi}{L}}\right]_{-L}^{L} - \int_{-L}^{L} F'(x)\frac{-\cos\frac{n\pi x}{L}}{\frac{n\pi}{L}}dx\right\} \\
=& \frac{L}{n\pi}\frac{1}{L}\int_{-L}^{L} F'(x)\cos\frac{n\pi x}{L}dx \\
=& \frac{L}{n\pi}\frac{1}{L}\int_{-L}^{L}\left[f(x)-\frac{1}{2}A_o\right]\cos\frac{n\pi x}{L}dx \\
=& \frac{L}{n\pi}\frac{1}{L}\left\{\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx - \frac{1}{2}A_o\frac{\left[\sin\frac{n\pi x}{L}\right]_{-L}^{L}}{\frac{n\pi}{L}}\right\} \\
=& \frac{L}{n\pi}A_n \qquad \text{for } n>0
\end{aligned}$$

Hence the Fourier series

$$F(x) = \frac{a_o}{2} + \sum_{n=1}^{\infty}\left[a_n\cos\frac{n\pi x}{L} + b_n\sin\frac{n\pi x}{L}\right] \tag{13.39}$$

becomes

$$\begin{aligned}
F(x) =& \left(\frac{1}{2}A_oL - \sum_{n=1}^{\infty} a_n(-1)^n\right) + \sum_{n=1}^{\infty}\left[a_n\cos\frac{n\pi x}{L} + b_n\sin\frac{n\pi x}{L}\right] \\
=& \frac{1}{2}A_oL + \sum_{n=1}^{\infty}\left\{a_n\left[\cos\frac{n\pi x}{L} - (-1)^n\right] + b_n\sin\frac{n\pi x}{L}\right\} \\
=& \frac{1}{2}A_oL + \sum_{n=1}^{\infty}\left\{-\frac{L}{n\pi}B_n\left[\cos\frac{n\pi x}{L} - (-1)^n\right] + \frac{L}{n\pi}A_n\sin\frac{n\pi x}{L}\right\} \qquad (13.40)
\end{aligned}$$

But $F(x) \equiv \int_{-L}^{x} f(x)dx - \frac{1}{2}A_o x$, so

$$\begin{aligned}
\int_{-L}^{x} f(x)dx =& \frac{1}{2}A_o(x+L) + \sum_{n=1}^{\infty}\left\{A_n\frac{L}{n\pi}\sin\frac{n\pi x}{L} - B_n\frac{L}{n\pi}\left[\cos\frac{n\pi x}{L} - (-1)^n\right]\right\} \\
=& \int_{-L}^{x}\frac{1}{2}A_o dx + \sum_{n=1}^{\infty}\left[A_n\int_{-L}^{x}\cos\frac{n\pi x}{L}dx + B_n\int_{-L}^{x}\sin\frac{n\pi x}{L}dx\right] \\
=& \text{Term-by-term integral of the Fourier series for } f(x).
\end{aligned}$$

$\int f(x) = \int$ fourier series for f	$f(x) =$ four. ser.	$\frac{\partial f(x)}{\partial x} = \frac{\partial}{\partial x}$ f. s.
$f(x)$piecewise continuous	$f(x)$continuous or piecewise $f'(x)$p.c.	$f(x)$periodic and continuous $f'(x)$p.c. $f''(x)$p.c.

13.12 Fourier Integral Representation

If $f(x)$ is piecewise smooth for $-L \leq x \leq L$, it has a complex Fourier series.

$$F(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\frac{\pi x}{L}} \qquad c_n \equiv \frac{1}{2L}\int_{-L}^{L} f(x) e^{-in\frac{\pi x}{L}} dx$$

which converges to $\frac{1}{2}[f(x+) + f(x-)]$ for $-L < x < L$.

We wish to consider what happens as $L \to \infty$. We cannot naively put $l = \infty$ for c_n because that gives $c_n = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)dx$ for all n, and the Fourier series becomes just $\sum_{n=-\infty}^{\infty} c_n$. Putting c_n in the series for $f(x)$:

$$\begin{aligned} f(x) &= \sum_{n=-\infty}^{\infty} \left[\frac{1}{2L}\int_{-L}^{L} f(x')\right] e^{i\frac{n\pi x}{L}} \\ &= \sum_{n=-\infty}^{\infty} \frac{1}{2L}\int_{-L}^{L} dx' f(x') e^{i\frac{n\pi}{L}(x-x')} \end{aligned} \tag{13.41}$$

Let $\Delta k \equiv \frac{\pi}{L}$. Then,

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{\Delta k}{2\pi}\int_{-L}^{L} dx' f(x') e^{i\,n\delta k(x-x')} \tag{13.42}$$

But

$$\lim_{\Delta k \to 0} \sum_{n \to -\infty}^{\infty} F(n\Delta k)\Delta k = \int_{-\infty}^{\infty} F(k)dk \tag{13.43}$$

Hence, as $L \to \infty$, $\Delta k \equiv \frac{\pi}{L} \to 0$. Fourier integral expression for $f(x)$:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' f(x') e^{ik(x-x')} \tag{13.44}$$

This proof is heuristic (suggestive, but not rigorous). The result can be written

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk F(k) e^{ikx} \tag{13.45}$$

where

$$F(k) \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx' f(x') e^{-ikx'} \qquad \text{Fourier transform of } f(x)$$

Before providing rigorously the Fourier integral theorem, we need to consider "improper integrals" of the form:

$$\begin{aligned} I(k) &= \int_{a}^{\infty} f(x,k)dx \\ &= \lim_{R\to\infty} \underbrace{\int_{a}^{R} f(x,k)dx}_{I_R(k)} \\ &= \lim_{R\to\infty} I_R(k) \end{aligned} \tag{13.46}$$

or

$$\begin{aligned} I(k) &= \int_{-\infty}^{\infty} f(x,k)dx \\ &= \lim_{R\to\infty} \int_{-R}^{R} F(x,k)dx \\ &= \lim_{R\to\infty} I_R(k) \end{aligned} \tag{13.47}$$

$I(k)$ is said to converge uniformly in k, for $A \le k \le B$, if given $\epsilon > o$, one can find Q, independent of k for $a \le k \le b$, such that

$$|I(k) - I_R(k)| < \epsilon \quad \text{for} \quad R > Q$$

13.13 M-Test for Uniform Convergence

If $|f(x,k)| \le M(x)$ for $A \le k \le B$ and if $\int_a^\infty M(x)$ exists, then $\int_a^\infty f(x,k)dx$ converges uniformly. A uniformly convergent improper integral $I(k)$ can be integrated under the integral sign:

$$\int_A^B dk \int_{-\infty}^{\infty} f(x,k)dx = \int_{-\infty}^{\infty} \left(\int_A^B f(x,k)dk \right) dx \tag{13.48}$$

These properties are analogous to those of a uniformly convergent infinite series:

$$\begin{aligned} S(k) &= \sum_{n=0}^{\infty} F_n(k) \\ &= \lim_{N\to\infty} \sum_{n=0}^{N} F_n(k) \end{aligned} \tag{13.49}$$

An important simpler example is

$$I(k) = \int_{-\infty}^{\infty} F(x)e^{ikx}dx \tag{13.50}$$

If $\int_{-\infty}^{\infty} |f(x)|dx$ exists, then $I(k)$ converges uniformly in k, since $|f(x)e^{ikx}| = |f(x)|$, so one can take $M(x) = |f(x)|$.

13.14 Fourier Integral Theorem

If $f(x)$ is piecewise smooth for all finite intervals, if $\int_{-\infty}^{\infty} |f(x)|dx$ exists, and if

$$F(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ikx}dx \tag{13.51}$$

then

$$f(x) \equiv \frac{1}{2}[f(x+) + f(x-)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)e^{ikx}dk \tag{13.52}$$

$$\begin{aligned} F\{\,\} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx}\{\,\} \\ F^{-1}\{\,\} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{-ikx}\{\,\} \end{aligned}$$

Proof: Reference: Dettman, Chapter 8, or Churchill.

Lemma 2 *Riemann's Lemma. If $f(x)$ is piecewise continuous for $a \leq x \leq b$, a and b finite, then* $\lim_{R\to\infty} \int_a^b f(x) \sin Rx\, d$
0

Proof: Since the integral can be split up into integrals of a continuous fct, Lemma 2 is true if it si true for a continuous $f(x)$, which we now assume. If we change the variable from x to t such that $Rx = Rt + \pi$, so $x = t + \frac{\pi}{R}$,

$$\int_a^b f(x) \sin Rx dx = \int_{a-\frac{\pi}{R}}^{b-\frac{\pi}{R}} f\left(t + \frac{\pi}{R}\right) \underbrace{\sin(Rt+\pi)}_{-\sin Rt} dt$$
$$= -\int_{a-\frac{\pi}{R}}^{b-\frac{\pi}{R}} f\left(t + \frac{\pi}{R}\right) \sin Rt\, dt \tag{13.53}$$

Hence, adding these expressions:

$$2\int_a^b f(x) \sin Rx\, dx = \int_a^b f(x) \sin Rx\, dx - \int_{a-\frac{\pi}{R}}^{b-\frac{\pi}{R}} f\left(x + \frac{\pi}{R}\right) \sin Rx\, dx$$
$$= -\int_{a-\frac{\pi}{R}}^{a} f\left(x + \frac{\pi}{R}\right) \sin Rx\, dx$$
$$- \int_a^{b-\frac{\pi}{R}} \left[f\left(x + \frac{\pi}{R}\right) - f(x)\right] \sin Rx\, dx$$
$$+ \int_{b-\frac{\pi}{R}}^{b} f(x) \sin Rx\, dx$$

$$2\left|\int_a^b f(x) \sin Rx\, dx\right| \leq \left|\int_{a-\frac{\pi}{R}}^{a} f\left(x + \frac{\pi}{R}\right) \sin Rx\, dx\right|$$
$$+ \left|\int_a^{b-\frac{\pi}{R}} \left[f\left(x + \frac{\pi}{R}\right) - f(x)\right]\right| + \left|\int_{b-\frac{\pi}{R}}^{b} f(x) \sin Rx\, dx\right|$$
$$\leq \frac{\pi}{R}M + \left|b - \frac{\pi}{R} - a\right| \left|f\left(x + \frac{\pi}{R}\right) - f(x)\right|_{max} + \frac{\pi}{R}M$$

for $a \leq x \leq b\frac{\pi}{R}$ where $|f(x)| \leq M$ for $a \leq x \leq b$. M is finite, and $\left|f\left(x + \frac{\pi}{R}\right) - f(x)\right|_{max} \to 0$ as $R \to \infty$ because $f(x)$ is continuous. Hence

$$\lim_{R\to\infty} 2\left|\int_a^b f(x) \sin Rx dx\right| = 0$$
$$\Rightarrow \lim_{R\to\infty} \int_a^b f(x) \sin Rx dx = 0$$

Lemma 3 *If $f(x)$ is piecewise smooth in any finite interval and $\int_{-\infty}^{\infty} |f(x)| dx < \infty$, then*

$$\lim_{R\to\infty} \int_{-T}^{T} f(x+t) \frac{\sin Rt}{t} dt = \frac{\pi}{2}[f(x+) + f(x-)] \qquad 0 < T \leq \infty$$

Proof: First consider finite T

$$
\begin{aligned}
I_T \equiv & \lim_{R\to\infty}\int_{-T}^{T} f(x+t)\frac{\sin Rt}{t}dt - \frac{\pi}{2}[f(x+)+f(x-)] \\
= & \lim_{R\to\infty}\int_{0}^{T} [f(x+t)+f(x-t)]\frac{\sin Rt}{t}dt - \frac{\pi}{2}[f(x+)+f(x-)]
\end{aligned}
$$

But

$$
\begin{aligned}
\lim_{R\to\infty}\int_0^T \frac{\sin Rt}{t}dt = & \lim_{R\to\infty}\int_0^{RT}\frac{\sin t'}{t'}dt' \\
= & \int_0^\infty \frac{\sin t}{t}dt \\
= & \frac{\pi}{2}
\end{aligned}
$$

as we showed last semester by contour integration.

Hence

$$
I_T = \lim_{R\to\infty}\int_0^T \left[\frac{f(x+t)-f(x+)}{t} + \frac{f(x-t)-f(x-)}{t}\right]\sin Rt\, dt
$$

=0 from Lemma 2, since the integrand is piecewise continuous for all finite $t \geq 0$

$$
\lim_{t\to 0}\left[\frac{f(x+t)-f(x+)}{t} + \frac{f(x-t)-f(x-)}{t}\right] = f'_R(x) - f'_L(x) \tag{13.54}
$$

which exists fince $f'(x)$ is piecewise continuous. This proves the Lemma for finite T. For $T=\infty$

But

$$
\int_{-\infty}^{\infty}|f(x+t)|dt = \int_{-\infty}^{\infty}|f(t)|dt
$$

so given any $\epsilon > 0$ can find T large enough so $\left(\int_{-R}^{-T} + \int_T^\infty\right) f(t)dt < \epsilon$

Hence

$$
\begin{aligned}
& \lim_{R\to\infty}\left|\int_{-\infty}^{\infty} f(x+t)\frac{\sin Rt}{t}dt - \frac{\pi}{2}[f(x+)+f(x-)]\right| \\
& < \epsilon + \underbrace{\lim_{R\to\infty}\left|\int_{-T}^{T} f(x+t)\frac{\sin Rt}{t}dt - \frac{\pi}{2}[f(x+)+f(x-)]\right|}_{0\text{, from proof for finite } T\text{, Lemma 2}} \\
& = 0,\ \epsilon \text{ arbitrary, since}
\end{aligned}
$$

Q.E.D.

$$
\Rightarrow \lim_{R\to\infty}\int_{-\infty}^{\infty} f(x+t)\frac{\sin Rt}{t}dt = \frac{\pi}{2}[f(x+)+fx-]
$$

Proof of the Fourier Integral Theorem:

$$
\begin{aligned}
\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)e^{ikx}dk = & \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x')e^{-ikx'}dx'\right\}e^{ikx} \\
= & \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\int_{-\infty}^{\infty} dx' f(x')e^{ik(x-x')} \\
= & \lim_{R\to\infty}\frac{1}{\sqrt{2\pi}}\int_{-R}^{R} dk\int_{-\infty}^{\infty} dx' f(x')e^{ik(x-x')}
\end{aligned}
$$

But $|f(x')e^{ik(x-x')}| = |f(x')|$ and $\int_{-\infty}^{\infty} dx'|f(x')| < \infty$, so the integral over x' converges uniformly in k, so the order of the integration can be exchanged.

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(x)e^{ikx}dk &= \lim_{R\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} dx'\, f(x')\int_{-R}^{R} dk\, e^{ik(x-x')} \\
&= \lim_{R\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} dx'\, f(x')\left[\frac{\sin k(x-x')}{(x-x')}\right]_{k=-R}^{k=R} \\
&= \lim_{R\to\infty}\frac{1}{\pi}\int_{-\infty}^{\infty} dx'\, f(x')\frac{\sin R(x-x')}{x-x'} \\
&= \lim_{R\to\infty}\frac{1}{\pi}\int_{-\infty}^{\infty} dt\, f(x+t)\frac{\sin Rt}{t} \\
&=\frac{1}{2}[f(x+)+f(x-)] \text{ from Lemma 3.} \qquad \text{Q.E.D.}
\end{aligned}$$

We note for future reference that the Fourier transform $F(k)$ of a piecewise smooth function $f(x)$ statisfying $\int_{-\infty}^{\infty}|f(x)|dx < \infty$ is bounded:

$$F(k) \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx$$

so

$$\begin{aligned}
|F(k)| \leq& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} |f(x)e^{-ikx}|dx \\
=& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} |f(x)|dx \\
=& B < \infty
\end{aligned}$$

since $\int_{-\infty}^{\infty}|f(x)|dx < \infty$

$$\Rightarrow |F(k)| \leq B < \infty$$

13.15 Examples of the Fourier Integral Theorem

$$f(x) = ce^{-\frac{x^2}{\sigma^2}}, \text{ called a gaussian function.} \tag{13.55}$$

$$\frac{1}{\sigma^2} = \lambda \qquad \sigma^2 = \frac{1}{\lambda} \qquad \sigma = \frac{1}{\sqrt{\lambda}}$$

$$
\begin{aligned}
F(k) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} c e^{-\frac{x^2}{\sigma^2}} e^{-ikx} dx \\
=& \frac{c}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{\sigma^2}} \left[x^2 + ik\sigma^2 x\right] dx \\
=& \frac{c}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{\sigma^2}} \left[x^2 + ik\sigma^2 x + \left(\frac{ik\sigma^2}{2}\right)^2 - \left(\frac{ik\sigma^2}{2}\right)^2\right] dx \\
=& \frac{c}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{\sigma^2}} \left(x + \frac{ik\sigma^2}{2}\right)^2 dx \, e^{-\frac{1}{\sigma^2}\frac{k^2\sigma^4}{4}} \\
=& \frac{c}{\sqrt{2\pi}} e^{-\frac{k^2\sigma^4}{4}} \underbrace{\left(\int_{-\infty}^{\infty} e^{-\frac{x^2}{\sigma^2}} \frac{dx}{\sigma}\right)}_{\sqrt{\pi}} \sigma \\
=& \frac{c\sigma}{\sqrt{2}} e^{-\frac{\sigma^2}{4}k^2}
\end{aligned}
$$

which is a gaussian function of k.

Note that

$$\int_{-\infty}^{\infty} f(x)dx = \sqrt{2\pi}F(0) = \sqrt{2\pi}\frac{c\sigma}{\sqrt{2}} = 1$$

if $c = \frac{1}{\sigma\sqrt{\pi}}$.

So $f(x) = \frac{1}{\sigma\sqrt{\pi}} e^{\frac{-x^2}{\sigma^2}}$ had $F(k) = \frac{1}{sqrt 2\pi} e^{\frac{-\sigma^2}{4}k^2}$

$$\Delta x \equiv \sigma \qquad \Delta k \equiv \frac{2}{\sigma} \Rightarrow \Delta x \Delta k = \sigma \frac{2}{\sigma} = 2, \text{ for all } \sigma \tag{13.56}$$

The narrower $f(x)$, the broader $F(k)$. This is typical of all functions and their Fourier transforms.

As $\sigma \to 0$, $f(x) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{x^2}{\sigma^2}}$ approaches the Dirac delta function, $\delta(x)$, which has the properties $\delta(x) = 0$ if $x \neq 0$, but $\int_{-\infty}^{\infty} \delta(x)dx = 1$, and

$$f(x) = \int_{-\infty}^{\infty} f(x')\delta(x'-x)dx'$$

if $f(x)$ is continuous at x. The last property follows from

$$\int_{-\infty}^{\infty} f(x')\delta(x'-x)dx' = \int_{x-\epsilon}^{x+\epsilon} f(x')\delta(x'-x)dx' = f(x) \underbrace{\int_{x-\epsilon}^{x+\epsilon} \delta(x'-x)dx'}_{1} = f(x)$$

The Fourier transform of $\delta(x - x_o)$ is

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x - x_o) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} e^{-ikx_o}$$

so the Fourier integral representation is:

$$\delta(x - x_o) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ck(x-x_o)} dk$$

This important result follows also from putting

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \tag{13.57}$$

in

$$\begin{aligned} f(x) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk \\ =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \right\} e^{ikx} dk \\ =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' f(x') e^{ck(x-x')} \\ =& \int_{-\infty}^{\infty} dx' f(x') \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik}(x-x') dk \right\}, \quad \text{exchanging order of integration} \\ =& \int_{-\infty}^{\infty} f(x') \delta(x'-x) dx \end{aligned}$$

$$\begin{aligned} \delta(x'-x) =& \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk \\ =& \frac{1}{2\pi} \int_{0}^{\infty} \cos k(x-x') dk \\ =& 12\pi \int_{-\infty}^{\infty} e^{ik(x'-x)} dk \end{aligned}$$

As another example, consider

$$f(x) = \begin{cases} e^{ik_o x}, & -\sigma \leq x \leq \sigma \\ 0, & x < -\sigma, \quad x > \sigma \end{cases} \tag{13.58}$$

$$\begin{aligned} F(k) =& \frac{1}{2\pi} \int_{-\sigma}^{\sigma} e^{ik_o} e^{ikx} dx \\ =& \frac{1}{2\pi} \int_{-\sigma}^{\sigma} e^{i(k-k_o)x} dx = \frac{1}{2\pi} \int_{-\sigma}^{\sigma} \cos(k-k_o)x dx \\ =& \frac{1}{2\pi} \frac{\sin(k-k_o)x}{(k-k_o)} |_{-\sigma}^{\sigma} = \sqrt{\frac{2}{\pi}} \frac{\sin(k-k_o)\sigma}{(k-k_o)} = \sigma \sqrt{\frac{2}{\pi}} \frac{\sin(k-k_o)\sigma}{(k-k_o)\sigma} \end{aligned}$$

$$\Delta x \Delta k = \sigma \frac{\pi}{\sigma} = \pi$$

13.16 Parseval's Theorem for Fourier Transforms

Suppose $f(x)$ and $g(x)$ are piecewise smooth for all finite intervals, and $\int_{-\infty}^{\infty} |f(x)| dx$ and $\int_{-\infty}^{\infty} |g(x)| dx$ exist, so $f(x)$ and $g(x)$ have Fourier integral representations with Fourier transforms $F(k)$ and $G(k)$ which are bounded, so in particular $|G(k)| < B$ for all k.

The Parseval theorem is that:

$$\int_{-\infty}^{\infty} g^*(x) f(x) dx = \int_{-\infty}^{\infty} G^*(k) F(k) dk \tag{13.59}$$

Proof:

$$\begin{aligned}\int_{-\infty}^{\infty} G^*(k)F(k)dk &= \int_{-\infty}^{\infty} dkG^*(k)\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx\right\}\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\left\{\int_{-\infty}^{\infty} f(x)G^*(k)e^{-ikx}dx\right\}\end{aligned}$$

But the integral over x converges uniformly in k, since

$$|f(x)G^*(k)e^{-ikx}| \leq |f(x)|B, \quad \equiv M(x)$$

and

$$\int_{-\infty}^{\infty} M(x)dx = B\int_{\infty}^{\infty} |f(x)|dx < \infty$$

Hence the order of integration can be changed:

$$\begin{aligned}\int_{-\infty}^{\infty} G^*(k)F(k)dk =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dxF(x)\left\{\int_{-\infty}^{\infty} G^*(k)e^{-ikx}dk\right\}\\ =& \int_{-\infty}^{\infty} dxF(x)\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} G(k)e^{ikx}dk\right\}^*\\ =& \int_{-\infty}^{\infty} dxf(x)g(x)^*, \quad \text{Q.E.D.}\end{aligned} \tag{13.60}$$

For the special case $g(x) = f(x)$,

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |F(k)|^2 dk \tag{13.61}$$

13.17 Convolution Theorem for Fourier Transforms

If $H(k) = G(k)F(k)$, where

$$G(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x)e^{-ikx}dx \quad \text{and} \quad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx,$$

then

$$\begin{aligned}h(x) =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} H(k)e^{ikx}dk\\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} G(k)F(k)e^{ikx}dk\\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x')e^{-ikx'}dx'\right\}F(k)e^{ikx}\\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\int_{-\infty}^{\infty} dx'g(x')e^{ik(x-x')}(k)\end{aligned} \tag{13.62}$$

The integral over x' converges uniformly in k, since

$$\int_{-infty}^{\infty} dx'|g(x')|$$

exists, and $|F(k)| \leq B$, so the order of integration can be exchanged.

$$\begin{aligned} h(x) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dk F(k) e^{ik(x-x')} g(x') \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx' g(x') \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ik(x-x')} dk \right\} \end{aligned} \quad (13.63)$$

$$h(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x') f(x-x') dx'; \quad \text{Called the Fourier Convolution of } f(x) \text{ and } g(x)$$

If we change the variable of integration to $x'' = x - x',\ dx'' = -dx'$

$$\begin{aligned} h(x) =& \frac{1}{\sqrt{2\pi}}\int_{\infty}^{-\infty} g(x-x'') f(x'') (-dx'') \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x'') g(x-x'') dx'' \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x') g(x-x') dx' \end{aligned} \quad (13.64)$$

Hence the convolution is symmetric in the two functions f and g. The significance of the convolution $h(x)$ is that it is the function whose Fourier transform is the product of the transforms of f and g.

$$F\{h(x)\} = \bar{h}(k) = \bar{g}(k)\bar{f}(k)$$

13.18 Fourier Sine and Cosine Transforms and Representations

$$F(k) \equiv \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)[\cos kx - \sin kx] dx$$

Hence, if $f(-x) = f(x)$, an even function,

Bibliography

(1) ARFKEN, G. B., AND WEBER, H. J. *Mathematical methods for physicists*, 5 ed. Academic Press, San Diego, 2001.

(2) BAMBERG, P., AND STERNBERG, S. *A course in mathematics for students of physics: 1*. Cambridge University Press, Cambridge, 1991.

(3) BAMBERG, P., AND STERNBERG, S. *A course in mathematics for students of physics: 2*. Cambridge University Press, Cambridge, 1991.

(4) CHOQUET-BRUHAT, Y., DEWITT-MORETTE, C., AND DILLARD-BLEICK, M. *Analysis, manifolds and physics. Part I: basics*, revised ed. North-Holland, Amsterdam, 1991.

(5) CHOQUET-BRUHAT, Y., AND DEWITT-MORETTE, C. *Analysis, manifolds and physics. Part II: 92 applications*. North-Holland, Amsterdam, 1989.

(6) ALLEN, M., AND TILDESLEY, D. *Computer Simulation of Liquids*. Oxford University Press, 1987.