Physics 164
Mathematics for Quantum Theory

What is this course about?

It could have been **Functional Analysis**:

i.e. unbounded operators in Hilbert Space

self Adjointness, Spectral Theorem

(Von Neumann)

Instead, Physics, rather than Mathematics will receive prior emphasis.

The Theory of Scattering

Really the same as microscopic physics, since all that we know about atoms, nuclei, particles, etc is learned in scattering experiments.

In a sense, encompasses all of Quantum Mechanics.

Topics

1. Review of Quantum Mechanics
2. Scattering Formalism $\begin{cases} \text{Time-dependent} \\ \text{Time-independent} \end{cases}$
3. Partial Wave Expansion
4. Complex Angular Momentum
5. Analytic Properties of the S-Matrix
6. Dispersion Relations
7. Inverse Scattering Problem

Recommended Text

J.R. Taylor, Scattering Theory

Prerequisites

Quantum Mechanics (Physics 143)

Mathematics: Linear Algebra
Complex Analysis? Analytic Function
Residue Theorem

Requirements

Problem Sets
Final Exam (Possibly Oral)

Physics 164

I. Quantum Mechanics

We will review the mathematical formulation of Quantum Mechanics. Many subtleties will be ignored

1. States are rays in a Hilbert Space $\mathcal{H}$.

- What is a Hilbert Space?
  - a) A vector space over $\mathbb{C}$.
  - b) Has an inner product (ψ, φ), i.e.
    - i) Positive $\quad (\psi,\psi) > 0$ if $\psi \neq 0$
    - ii) $(\psi, a\varphi + b\varphi') = a(\psi,\varphi) + b(\psi,\varphi')$
    - iii) $(\varphi, \psi) = (\psi, \varphi)^*$
  - c) $\|\psi\| = (\psi,\psi)^{1/2}$ defines a norm, and the space is <u>complete</u> in this norm (All Cauchy sequences have limits)

  ψ_n Cauchy: Given ϵ, $\exists N$ s.t. $\|\psi_n - \psi_m\| < \epsilon$ for $n,m > N$

Important example:

Square integrable functions $L^2(\mathbb{R}^N)$

i.e. $\int d^N x \, |\psi(\vec{x})|^2 < \infty$

(This integral is defined w.r.t. Lebesgue measure, but we will not go into details of measure theory in this course. Completeness is the key property of L^2. It allows us to do Fourier analysis, i.e. guarantees that eigenfunction expansions converge.)

Define: $(\varphi, \psi) = \int d^N x \, \varphi^*(\vec{x}) \psi(\vec{x})$

- A *state* is a complete description of a physical system.
- A *Ray* is a vector of unit length and arbitrary phase.

  Superposition of states is also a physically realizable state. Of course, relative phases are important when we superpose states (interference)

2. Observables are self-adjoint operators

- An *observable* is a property of a physical system which can be measured: Position, Momentum, Energy, Angular momentum
- An *operator* is a linear transformation on $\mathcal{H}$

$$A: \psi \to A(\psi)$$
$$A(a\psi + b\varphi) = aA(\psi) + bA(\varphi)$$

- The *adjoint* of an operator is defined by

$$(\varphi, A\psi) = (A^{+}\varphi, \psi) \qquad \forall \varphi, \psi$$

- A is *self-adjoint* if $A = A^{+}$ (or hermitian)
  (We are ignoring a subtlety here; see below)

  Example: The position operator on $L^2(\mathbb{R})$

$$X: \psi(x) \to x\,\psi(x)$$
$$(\varphi, X\psi) = \int dx\, \varphi^*(x)(x\psi(x)) = \int dx\,(x\varphi(x))^* \psi(x) = (X\varphi, \psi)$$

$$f(X): \psi(x) \to f(x)\psi(x)$$

  Momentum Operator $P = -i\frac{\partial}{\partial x}$ $(\hbar = 1)$

$$(\varphi, P\psi) = \int dx\, \varphi^*\left(-i\frac{\partial}{\partial x}\psi\right) = \int dx \left(-i\frac{\partial}{\partial x}\varphi\right)^* \psi \quad \text{(integrate by parts)}$$
$$= (P\varphi, \psi)$$

  or $f(P)$ e.g. $\frac{1}{2}P^2$ or $\frac{1}{2}P^2 + V(x)$

If A, B are self-adjoint, so is $A+B$
and $[(AB)^+ = B^+A^+]$ $\quad AB+BA \quad i(AB-BA)$

The subtlety: Domains

If $\psi \in L^2(\mathbb{R})$, $x\psi$ need not be. E.g. $\psi = \frac{cx}{x^2+1}$.

X is defined on a domain $D \subset \mathcal{H}$

We can choose D dense in $\mathcal{H}$.

E.g. $C_0^\infty(\mathbb{R})$ - infinitely differentiable, compact support - is dense in $L^2(\mathbb{R})$

self-adjoint really means A and A^+ have same domain

- The Spectral Theorem

The key property of self-adjoint operators in a finite-dimensional vector space is: they can be diagonalized, i.e. have an orthonormal basis of eigenvectors, and real eigenvalues

$$A = \sum_n |a_n\rangle a_n \langle a_n| \quad \text{Projection operator}$$

Projection onto Eigenspaces where A acts like multiplication.

$\langle a_n|$ is a linear functional

The generalization of this statement to an infinite dimensional Hilbert space must be stated carefully.

A self-adjoint operator A can be represented

$$A = \int_{\mathbb{R}} a \, dP_a \qquad \mathbb{1} = \int_{\mathbb{R}} dP_a$$

dP_a is a "projection valued measure"

with any interval $\Omega \subset \mathbb{R}$ it associates an orthogonal projection P_Ω

i.e. $\quad P^2 = P$, $\quad P = P^+$

i.e. P is the identity on its range, and zero on the space $\perp$ to range

$P(P\psi) = P\psi$

$(\varphi, P\psi) = 0 \Rightarrow (P\varphi, \psi) = 0$

The support of dP_a is the spectrum of A

E.g. for position operator $dP_{[a,b]}$ picks out wavepackets w/ support on $[a,b]$ - Spectrum is $\sigma(X) = \mathbb{R}$

If the measure dP_a has its support on discrete points only we may use the physicists notation

$$A = \sum_n |n\rangle a_n \langle n| , \quad \text{or} \quad \int da\, |a\rangle a \langle a|$$

and say that A has a basis of eigenvectors

But, in general, this statement is too careless if dP_a is continuous there need not be an eigenstate in $\mathcal{H}$ of A w/ eigenvalue a. Physicists speak of "improper eigenvectors" — this is just another way of saying that

$$A = \int_R a\, dP_a .$$

Example. Fourier transform "diagonalizes" $P = -i\frac{\partial}{\partial x}$

$$P\psi = -i\frac{\partial}{\partial x}\psi = \int dp\, p\, e^{ipx}\, \tilde{\psi}(p) \quad \text{— Spectral representation}$$

$$\tilde{\psi}(p) = \frac{1}{2\pi}\int dx\, e^{-ipx}\psi(x)$$

This is well defined, but the eigenfunction e^{ipx} of P is not square integrable.

(Projection picks out all wave packet states with given momentum spread.)

3. The outcome of a measurement of A is an element of the spectrum of A.

For a state ψ, measurement has a probability distribution

$$(\psi, dP_a \psi) \quad \text{or} \quad da\, \langle\psi|a\rangle\langle a|\psi\rangle$$

(Probability that measurement gives a value in the interval da)

Example - Position operator

$$(\psi, dP_x \psi) = dx\, |\psi(x)|^2$$

Expectation value of measurement is

$$\langle A\rangle_\psi = \int_{\mathbb{R}} a\, (\psi, dP_a \psi) = \int da\, a |\langle\psi|a\rangle|^2$$

4. Dynamics (time-translation) is generated by a self-adjoint Hamiltonian H.

- Consider the Schrodinger Picture

time evolution of states is governed by $U(t)$ - linear operator

$$\psi(t) = U(t)\,\psi(0)$$

what properties ought U to have?

a) $U(0) = \mathbb{1}$

b) U is invertible $\quad U(t)^{-1} = U(-t)$

Every state at time t evolved from some unique state at time 0

c) $U(t)$ is unitary - it must conserve probability

A physical requirement is that the probabilities of all possible outcomes of a measurement of an observable A must sum to 1 at any time t, and therefore

why can't time evolution be antiunitary? See p 1.9

$$\|\psi(t)\|^2 = \int da\, |\langle \psi(t)|a\rangle|^2 = \int da\, |\langle \psi(0)|a\rangle|^2 = \|\psi(0)\|^2$$

(if eigenstates $|a\rangle$ are a complete "basis")

For any $\psi \in \mathcal{H}$ we want $(U\psi, U\psi) = (\psi,\psi) = (\psi, U^{+}U\psi)$

In particular consider $\psi = \varphi + \varphi'$

$\psi' = \varphi + i\varphi'$

$$(\varphi+\varphi', \varphi+\varphi') = (\varphi+\varphi', U^{+}U(\varphi+\varphi'))$$

$$(\varphi+i\varphi', \varphi+i\varphi') = (\varphi-i\varphi', U^{+}U(\varphi-i\varphi'))$$

subtract: $(\varphi',\varphi) + (\varphi,\varphi') - i(\varphi,\varphi') + i(\varphi',\varphi) +$

$$= (\varphi, U^{+}U\varphi') + (\varphi', U^{+}U\varphi) - i(\varphi, U^{+}U\varphi') + i(\varphi', U^{+}U\varphi)$$

This eqn has the form $\quad \mathrm{Re}\, z - \mathrm{Im}\, z = \mathrm{Re}\, y - \mathrm{Im}\, y \qquad z = (\varphi',\varphi)$, $\; y = (\varphi', U^{+}U\varphi)$

Taking $\psi' = \varphi - i\varphi'$ we get $\quad \mathrm{Re}\, z + \mathrm{Im}\, z = \mathrm{Re}\, y + \mathrm{Im}\, y$

$$\Rightarrow \mathrm{Re}\, z = \mathrm{Re}\, y \text{ and } \mathrm{Im}\, z = \mathrm{Im}\, y \Rightarrow$$

$$(\varphi',\varphi) = (\varphi', U^{+}U\varphi) \Rightarrow U^{+}U = \mathbb{1}$$

Because U is invertible it follows that $UU^{+} = \mathbb{1}$

$$(UU^{+}U = U \Rightarrow UU^{+} = \mathbb{1})$$

A phase here can be absorbed

d) $U(t)U(s) = U(t+s)$

(U is a unitary representation of addition of real nos.)

$$\begin{tikzcd} \bullet \arrow[r, "t"] \arrow[rr, bend right, "t+s"'] & \bullet \arrow[r, "s"] & \bullet \end{tikzcd}$$

e) $U(t)$ is a continuous function of t — Requires that we specify topology (strong limits)

(We will actually assume that it is differentiable) i.e. $0 = \lim_{\Delta t \to 0} \left\| \left[\frac{U(t+\Delta t) - U(t)}{\Delta t} - U'(t) \right] \psi \right\|$ for all $\psi \in \mathcal{H}$

Claim: It follows that $\boxed{U(t) = e^{-itH}}$, where H is self adjoint. (This is a general property of one-parameter unitary group representations — they have self-adjoint generators)

Proof/ $\frac{d}{ds} U(t+s) = \frac{d}{dt} U(t+s) = \left[\frac{d}{dt} U(t)\right] U(s)$

Let $t \to 0 \Rightarrow \frac{d}{ds} U(s) = -iH\, U(s)$

where $-iH = \frac{d}{dt} U(t)\Big|_{t=0}$

i) H is self-adjoint

$$-iH = \lim_{t\to 0} \frac{U(t) - U(0)}{t} = \lim_{t \to 0} \frac{U(-t) - U(0)}{-t} = -(-iH)^{+} = -iH^{+}$$

ii) $U(t) = e^{-iHt}$ solves the differential equation <u>formally</u>, but how is it <u>defined</u>?

- If H is bounded, the power series converges in norm
- If H has a spectral representation, we define

$$f(H) = \int_{\mathbb{R}} f(h)\, dP_h \,, \quad e^0 = \mathbb{1} \text{ if } \int dP_h \text{ is } \underline{\text{complete}}$$

For this purpose, having a spectral representation is as good as having a basis of eigenvectors

iii) Uniqueness — we must show that there is only one solution to $\frac{dU}{dt} = -iHU$ with $U(0) = \mathbb{1}$

For any φ, set $\chi(t) = (U(t) - e^{-iHt})\varphi$

$$\Rightarrow \frac{d\chi}{dt} = -iH\chi(t)$$

$$\frac{d}{dt} \|\chi\|^2 = (-iH\chi, \chi) + (\chi, -iH\chi) = 0$$

i.e. χ has constant norm and $\chi(0) = 0 \Rightarrow \chi(t) = 0$

$$\Rightarrow U - e^{-iHt} = 0. \quad \text{QED}$$

Thus, in the Schrödinger Picture
$$\psi(t) = e^{-iHt}\psi(0) \text{ or } \boxed{i\frac{d}{dt}\psi(t) = H\psi(t)}$$
— Schrödinger Equation

• Another view of dynamics, Heisenberg Picture

Suppose states are viewed as fixed, but operators evolve

Physics must be the same:

we define $\psi_H = e^{iHt}\psi_S(t) = \psi_S(0)$

and require $\langle \psi_H | a_H(t) \rangle = \langle \psi_S(t) | a_S \rangle$

where $A_S = \int da_S |a_S\rangle a_S \langle a_S|$

$A_H = \int da_H |a_H(t)\rangle a_H \langle a_H(t)|$

$\Rightarrow |a_H(t)\rangle = e^{itH}|a_S\rangle$ or $A_H = e^{itH} A_S e^{-itH}$

Now we have completed our brief overview of the mathematical formulation of Quantum Mechanics

The fundamental mathematical problem is:

Given Hamiltonian H, what dynamics does it define.

A partial answer is found if we determine

5. The Spectrum (of H)

Before, we defined the spectrum of a self-adjoint operator as the support of its projection valued measure

A more general definition will be useful to us.

• First - we review the finite dimensional case: the spectrum of a matrix is the set of its eigenvalues

spectrum of $M = \{ \lambda \mid \det(\lambda 1\!\!1 - M) = 0 \}$

(the roots of the characteristic equation)

- To generalize to infinite-dimensional spaces (including unbounded operators) we define...

Resolvent set of $M = \rho(M) = \{\lambda \mid \lambda\mathbb{1} - M$ is a bijection (from its domain onto $\mathcal{H}$) with a bounded inverse$\}$

In fact, if Range$(\lambda - M) = \mathcal{H}$, inverse is automatically bounded

$G_M(\lambda) = R_\lambda(M) = (\lambda - M)^{-1}$ = "Resolvent of M at λ" or "Green's Operator"

If $\lambda \in \mathbb{C}$ is not in $\rho(M)$, then it is in $\sigma(M)$, The spectrum of M

$$\sigma(M) = \{\lambda \mid \lambda \notin \rho(M)\}$$

$\|A\| = \sup \frac{\|A\psi\|}{\|\psi\|}$

$\|A^{-1}\| = \sup \frac{\|\psi\|}{\|A\psi\|}$

If $= \infty$, $\exists$ sequence ψ_n s.t. $\|\psi_n\| = 1$ and $\|A\psi_n\| \to 0$; this has a limit point ψ, $A\psi = 0$

An important theorem, which we will apply extensively later in the course is

Thm: The resolvent R_λ ($G(z)$) is an analytic function of λ on the resolvent set ρ.

It suffices to show that for $\lambda_0 \in \rho$, R_λ has a convergent power series expansion about λ_0

Formally, we may show this as follows

$$G_M(z) = R_\lambda = \frac{1}{\lambda - M} = \frac{1}{\lambda - \lambda_0 + \lambda_0 - M} = \frac{1}{\lambda_0 - M}\left[1 - \frac{\lambda_0 - \lambda}{\lambda_0 - M}\right]^{-1} = \frac{1}{\lambda_0 - M}\sum_{n=0}^{\infty}\left(\frac{\lambda_0 - \lambda}{\lambda_0 - M}\right)^n$$

This series converges uniformly for $(\lambda_0 - \lambda)\|R_{\lambda_0}\| < 1 \Rightarrow R_\lambda$ analytic in a disc about λ_0

spectrum = points of nonanalyticity of R_λ.

~~There are two convenient ways of~~ subdividing the spectrum

1 a) If M has a (normalizable) eigenvector with eigenvalue λ, λ is in point spectrum of M

b) λ is in "residual spectrum" if Ran$(\lambda - M)$ not dense in $\mathcal{H}$, but it is not in point spectrum

$\}$ not exhaustive

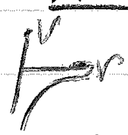
~~5.) The spectrum of the position operator is all residual spectrum of $\mathbb{R}$ - it has no eigenfunctions (the δ function is not in L^2)~~

2. a) $\sigma_{essential} = \{\lambda \mid \dim \operatorname{Ran} P_{\lambda-\epsilon,\lambda+\epsilon} = \infty \ \forall \epsilon > 0\}$
   b) $\sigma_{discrete} = \{\lambda \mid \dim \operatorname{Ran} P_{\lambda-\epsilon,\lambda+\epsilon} < \infty \ \forall \epsilon > 0\}$

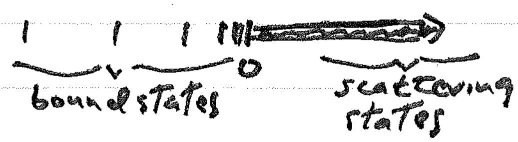
It is a theorem that
$\lambda \in \sigma_{discrete}$ iff a) λ is isolated
b) λ is an eigenvalue of finite multiplicity

(Square well potential in one dim)

<u>A typical Hamiltonian</u>: Hydrogen Atom (on $L^2(\mathbb{R}^3)$)



$$H = -\tfrac{1}{2}\Delta - \frac{e^2}{r}$$



Discrete Spectrum = Bound States
Essential Spectrum = Scattering States

Central Problems:
- Find Bound State Energies (H atom, Harmonic oscillator, etc)
- Asymptotic $t \to \pm\infty$ behavior

  Spectral measure for $E>0$ in H atom determines this scattering behavior

(i.e. we want to <u>diagonalize</u> H; find its spectral representation)

Note - point spectrum can be embedded in $\sigma_{essential}$

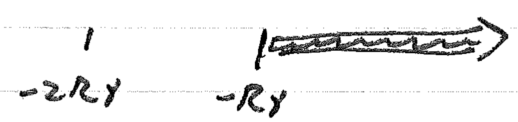
E.g. He atom (on $\mathbb{R}^6$) w/o e^-e^- interaction

$$H = -\tfrac{1}{2}\Delta_1 - \tfrac{1}{2}\Delta_2 - \frac{e^2}{r_1} - \frac{e^2}{r_2}$$

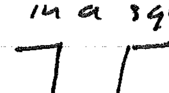
Bound Energies
$$E_1 = \frac{-Z^2 Ry}{n_1^2} \qquad E_2 = \frac{-Z^2 Ry}{n_2^2} \qquad (Ry = \tfrac{1}{2}e^4)$$

$\Rightarrow$ continuum begins at $-Ry$ (ionized)

but $n_1 = n_2 = 2$ is bound state with $E = -\tfrac{1}{2}Ry$



Or... Two particles in a square well.



Further Remarks:

Can time evolution be represented by an antiunitary operator?

Thm (Wigner) Suppose $\psi \to \psi'$ is a mapping which is 1-1 up to phases for all vectors of unit length

i.e. a 1-1 mapping of projections $|\psi\rangle\langle\psi| \to |\psi'\rangle\langle\psi'|$

and suppose $|(\phi, \psi)| = |(\phi' \psi')|$

Then $\exists$ T which is either unitary or antiunitary such that

$$\psi' = T\psi$$

- Thus, if we demand $|(\phi(0), \psi(0))| = |(\phi(t), \psi(t))|$ then time evolution operator $U(t)$ is either unitary or antiunitary
- This $U(t)$ is determined up to an overall phase for if $V(t)$ also had the desired property

$$U(t)|\phi\rangle\langle\phi|U(t)^+ = V(t)|\phi\rangle\langle\phi|V(t)^+$$

$$\Rightarrow \quad U(t)\phi = e^{ia}V(t)\phi$$

$$U(t)\psi = e^{ib}V(t)\psi$$

But $a=b$, because

$$U(t)(\phi+\psi) = e^{ic}V(t)(\phi+\psi)$$

Hence $\quad U(t) = e^{ia}V(t)$

- Now we also demand

$$U(t+s) = \omega(t,s)\,U(t)U(s)$$

↖ a phase factor

But $U(t+s)$ is unitary whether $U(t)$ and $U(s)$ are unitary or antiunitary

Thus all $U(t)$ must be unitary

- Finally we can get rid of the phase $\omega(t,s)$ (Wigner Ann Math 40, 149 (1939)) by absorbing it in U. $\exists\ \tilde{U}(t) = e^{ib(t)}U(t)$ such that

$$\tilde{U}(t+s) = \tilde{U}(t)\tilde{U}(s)$$

II. Time-Dependent Scattering Formalism

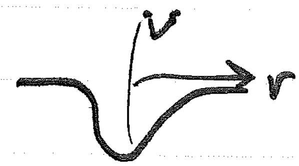
A. Asymptotic States and Wave Operators

Electromagnetic Scattering:
(e.g. by dust particle)

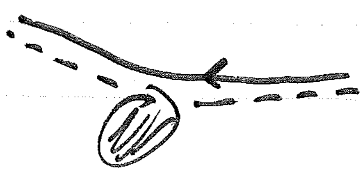
Incoming plane wave,
outgoing spherical wave

$\vec{E} = \vec{E}_0 e^{i\vec{k}\cdot\vec{r}} + \frac{\vec{E}_{scat}}{r} e^{ikr}$

"Scattering Theory" concerns asymptotic $r \to \infty$ behavior of fields.



Classical Scattering:
By a fixed target;
A potential which $\to 0$ as $r \to \infty$
"Scattering Theory" concerns orbits of unbound particles – in particular, the asymptotes of these orbits as $t \to \pm\infty$



Quantum Mechanics:
Occupies a middle ground

- we measure positions, momenta of particles distant from scattering center.
- But states are described by wave functions.
- plane waves are not normalizable ($\notin \mathcal{H}$). Instead, we must consider time evolution of wave packets. We will need to do some work before we can justifying speaking of the scattering of momentum-eigenstates".

Scattering
We consider $H = H^0 + V$

H^0 = free particle Hamiltonian
V = perturbation which is in some sense localized, so we can say

$H \to H^0$ as $r \to \infty$. Hence we consider wave packets propagating freely as $t \to \pm\infty$

In and Out States

We must generalize the classical notion of an asymptote for wave packets

First we define orbits in $\mathcal{H}$: $\{\psi(t) = U(t)\psi(0)\}$
These are in 1-1 correspondence with $\mathcal{H}$; i.e. are labeled by states at $t=0$

We want to consider "asymptotes" which are orbits evolving according to the free dynamics $U^0(t) = e^{-iH_0 t}$ and approach the actual orbits evolving according to $U(t) = e^{-iHt}$ as $t \to \pm\infty$

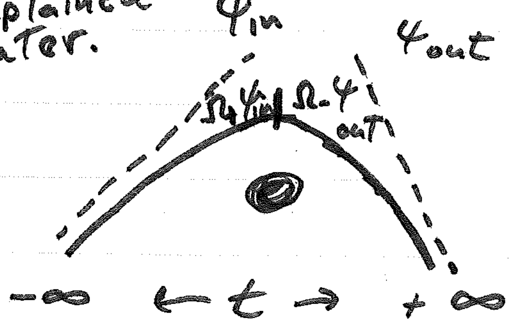
$$U(t)\psi(0) \longrightarrow U^0(t)\psi_{in}(0) \quad \text{as } t \to -\infty$$
$$U(t)\psi(0) \longrightarrow U^0(t)\psi_{out}(0) \quad \text{as } t \to +\infty$$

This is a mapping of actual orbits to free orbits, but, since orbits are in 1-1 corresponce with states in $\mathcal{H}$, it can be viewed as a mapping: $\mathcal{H} \to \mathcal{H}$

Therefore, let us define Wave Operators (or Møller Wave Operators) by

$$\begin{cases} \Omega_+ = \lim_{t\to-\infty} U(t)^\dagger U^0(t) & \psi = \Omega_+\psi_{in} \\ \Omega_- = \lim_{t\to+\infty} U(t)^\dagger U^0(t) & \psi = \Omega_-\psi_{out} \end{cases}$$

The perverse choice of sign convention will be explained later.



E.g. Ω_+ take asymptote $U^0(t)\psi_{in}$ back to $t=-\infty$, then brings it home again using full dynamics

Existence of Wave Operators

A central problem of scattering theory is to prove, for a given V. that $\Omega_\pm$ exist, i.e., the existence of asymptotes.

We will sketch the proof for $\mathcal{H} = L^2(\mathbb{R}^3)$ and V a square integrable function $\int d^3x\, |V|^2 < \infty$

we wish to show $\lim_{t\to\mp\infty} U(t)^\dagger U^0(t) = \Omega_\pm$ exists

i.e. $\lim_{t\to\mp\infty} U(t)^\dagger U^0(t)\, \psi_{\substack{in\\out}}$ exists for any $\psi_{\substack{in\\out}} \in \mathcal{H}$

(This is called a strong operator limit.)

i) **Lemma** : Consider a differentiable function $\psi(t): \mathbb{R} \to \mathcal{H}$

(Differentiable means $\exists\, \psi'(t)$ such that
$$\lim_{\epsilon\to 0} \left\| \frac{\psi(t+\epsilon) - \psi(t)}{\epsilon} - \psi'(t) \right\| = 0\ )$$

$\lim_{t\to\infty} \psi(t)$ exists if $\int_0^\infty d\tau \left\|\frac{d\psi}{d\tau}\right\| < \infty$

Proof

Because $\mathcal{H}$ is complete it suffices if
$\|\psi(t) - \psi(t')\| < \epsilon$ for $t, t' > T$
or $\left\|\int_{t'}^{t} \frac{d\psi(\tau)}{d\tau} d\tau\right\| < \epsilon$

But $\|\sum \psi_n\| \le \sum \|\psi_n\| \Rightarrow$ (Triangle $\neq$)

$$\left\|\int_{t'}^{t} \frac{d\psi(\tau)}{d\tau} d\tau\right\| \le \int_{t'}^{t} \left\|\frac{d\psi(\tau)}{d\tau}\right\| d\tau < \epsilon$$
if $\int^\infty d\tau \left\|\frac{d\psi}{d\tau}\right\| < \infty$.

Because of the lemma, it is enough to show

$$\int_0^\infty d\tau \left\| \frac{d}{d\tau}\left(U(\tau)^{+}U^{0}(\tau)\right)\psi_{out}\right\| < \infty \quad \text{to show } \Omega_- \text{ exists.}$$

$$\frac{d}{d\tau}U(\tau)^{+}U^{0}(\tau) = U(\tau)^{+}i(H-H^{0})U^{0}(\tau) = i\,U(\tau)^{+}VU^{0}(\tau)$$

$$\text{and } \quad \|iU(\tau)^{+}VU^{0}(\tau)\psi_{out}\| = \|VU^{0}(\tau)\psi_{out}\|$$

because $U(\tau)$ is unitary

$\therefore$ We must show

$$* \quad \int_0^\infty d\tau\, \|VU^{0}(\tau)\psi_{out}\| < \infty \quad \text{for all } \psi_{out} \in \mathcal{H}$$

ii) We can work out explicitly how $U^{0}(\tau)$ acts on a <u>Gaussian</u> wave packet. Suppose we show * for ψ_{out} Gaussian. It is a fact (that we will not prove) that any $\psi_{out} \in \mathcal{H}$ can be arbitrarily well approximated by a finite superposition of Gaussians.

For any ψ we know $\|\psi - \psi_g\| < \epsilon$ for ψ_g = superposition of gaussians

and $\|A(t)\psi_g - A(t')\psi_g\| < \epsilon'$ for $t, t' > T$

$A = U(t)^{+}U^{0}(t)$

Thus $\|A(t)\psi - A(t')\psi\|$

$$\leq \|A(t)(\psi-\psi_g)\| + \|A(t)\psi_g - A(t')\psi_g\| + \|A(t')(\psi-\psi_g)\|$$

$$< \epsilon/3 + \epsilon/3 + \epsilon/3 = \epsilon \quad (\text{because } \|A(t)\psi - \psi_g\| = \|\psi - \psi_g\|)$$

Therefore, it suffices to show * for Gaussians

iii) Consider $\psi(\vec{x},0) = \exp[-\vec{x}^2/2\sigma^2]$

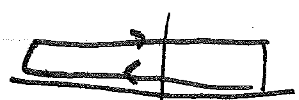
Lets solve $i\dfrac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi$ & find $\psi(\vec{x},t)$.

Fourier transform in $\vec{x}$:

$$\frac{\partial}{\partial t}\tilde{\psi}(\vec{p},t) = -\frac{i}{2}p^2\tilde{\psi}(\vec{p},t) \Rightarrow \tilde{\psi}(\vec{p},t) = e^{-\frac{i}{2}p^2 t}\tilde{\psi}(\vec{p},0)$$

$$\tilde{\psi}(\vec{p},0) = \int d^3x\, e^{-i\vec{p}\cdot\vec{x}} e^{-\vec{x}^2/2\sigma^2} = \int d^3x\, e^{-(\vec{x}+i\vec{p}\sigma^2)^2/2\sigma^2} e^{-p^2\sigma^2/2}$$

$$= (\sqrt{2\pi}\,\sigma)^3 e^{-p^2\sigma^2/2}$$



(same as integrating on real line)

$$\psi(\vec{x},t) = \int\frac{d^3p}{(2\pi)^3} e^{i\vec{p}\cdot\vec{x}}\tilde{\psi}(\vec{p},t)$$

$$= \int\frac{d^3p}{(2\pi)^{3/2}} e^{i\vec{p}\cdot\vec{x}}\sigma^3 e^{-\frac{i}{2}p^2 t} e^{-p^2\sigma^2/2}$$

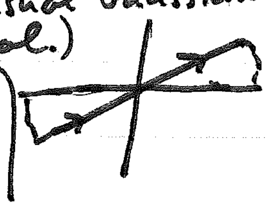
$$= \frac{\sigma^3}{(2\pi)^{3/2}}\int d^3p\, \exp\left[-\tfrac{1}{2}p^2(\sigma^2+it) + i\vec{p}\cdot\vec{x}\right]$$

complete the square again

$$\exp\left[-\tfrac{1}{2}(\sigma^2+it)\left(\vec{p}-\frac{i\vec{x}}{\sigma^2+it}\right)^2 - \frac{1}{2}\frac{x^2}{\sigma^2+it}\right]$$

$$\psi(\vec{x},t) = \frac{\sigma^3}{(\sigma^2+it)^{3/2}} e^{-\frac{1}{2}x^2/(\sigma^2+it)}$$

(Analytic continuation of the usual Gaussian integral.)



$$\psi(\vec{x},t) = \frac{1}{\left(1+\frac{it}{\sigma^2}\right)^{3/2}}\exp\left[-\frac{1}{2}\frac{x^2}{\sigma^4+t^2}(\sigma^2-it)\right]$$

$$\Rightarrow \boxed{|\psi(\vec{x},t)|^2 = \left(\frac{1}{1+\frac{t^2}{\sigma^4}}\right)^{3/2}\exp\left[-x^2/(\sigma^2+t^2/\sigma^2)\right]}$$

The significant thing is that the wave packet spreads — Max decreases like $1/t^3$.

This is because packet has indefinite momentum. It describes a collection of particles with different velocities.

It is left as an exercise to show that

$$\psi(\vec{x},0) = \exp\left[-(\vec{x}-\vec{a})^2/2\sigma^2 + i\vec{k}\cdot\vec{x}\right]$$

$$\Rightarrow \boxed{|\psi(\vec{x},t)|^2 = \frac{1}{(1+t^2/\sigma^4)^{3/2}} \exp\left[\frac{(\vec{x}-\vec{a}-\vec{k}t)^2}{\sigma^2+t^2/\sigma^2}\right]}$$

Wave packet <u>moves</u> <u>and</u> <u>spreads</u>

iv) Now we can complete the proof:

$$\|VU^0(\tau)\psi_{out}\|^2 = \int d^3x\, |V|^2 |\psi^0_{out}(\tau)|^2$$

$$\leq \left(\int d^3x\, |V|^2\right) \times \sup_{\vec{x}} |\psi^0_{out}(\tau)|^2$$

$$= \frac{C}{(1+t^2/\sigma^4)^{3/2}} \quad \text{because } V \in L^2(\mathbb{R}^3)$$

Hence $\int_0^\infty d\tau\, \|VU^0(\tau)\psi_{out}\| \leq \text{const} \int_0^\infty (1+t^2/\sigma^4)^{-3/2} dt < \infty$

QED

We have proved existence of

$$\lim_{t\to\mp\infty} U(t)^+ U^0(t) = \Omega_\pm \quad \text{Møller Wave Operators}$$

for $V = H - H^0$ a square-integrable function

By doing more work, we could have shown $\Omega_\pm$ exist for

$$V = V_2 + V_{3-\epsilon} \qquad \begin{array}{l} V_2 \in L^2(\mathbb{R}^3) \\ V_{3-\epsilon} \in L^{3-\epsilon}(\mathbb{R}^3) \quad 0<\epsilon\leq 1 \end{array}$$

i.e. $\int d^3x\, |V_{3-\epsilon}|^{3-\epsilon} < \infty$

Thus we can prove existence of the wave operators for

$$V < \frac{c}{r^{3/2}} \quad \text{as } r \to 0$$

$$V < \frac{c'}{r^{1+\epsilon}} \quad \text{as } r \to \infty \qquad \text{(Does not include Coulomb potential)}$$

Properties of the Wave Operators

$$\Omega_\pm = \lim_{t \to \mp\infty} U(t)^\dagger U^0(t) \quad \text{- a limit of a unitary operator.}$$

Must $\Omega_\pm$ therefore be unitary?

<u>No</u>, not in general

It <u>is</u> true that $\lim_{t\to\mp\infty} \| U(t)^\dagger U^0(t) \psi \| = \lim \|\psi\| = \|\psi\|$

or $\|\Omega_\pm \psi\| = \|\psi\|$

$\Omega_\pm$ is an <u>isometry</u>

On a finite dimensional space, an isometry is necessarily unitary.

In infinitely dimensional case, we can conclude

$$(\Omega\psi, \Omega\psi) = (\psi, \Omega^\dagger\Omega\psi) = (\psi, \psi)$$

$$\Rightarrow \Omega^\dagger\Omega = \mathbb{1}$$

But we cannot conclude that $\Omega\Omega^\dagger = \mathbb{1}$, unless Ω is invertible.

i.e. an isometry can be a unitary mapping from $\mathcal{H}$ onto a <u>subspace</u> of $\mathcal{H}$

Is there reason to doubt that $\Omega_\pm$ are actually unitary?

i.e. does every orbit have in and out asymptotes?

$$U(t)\psi \to U^0(t)\psi_{\substack{in\\out}} \quad \text{for all } \psi?$$

Even in classical mechanics the answer is no - there are bound orbits.

But if H has reasonable scattering behavior, we would expect that ...

a) Every orbit with an in asymptote has an out asymptote, and vice versa

$$\operatorname{Ran}\Omega_+ = \operatorname{Ran}\Omega_- = \mathcal{R} = \text{"scattering states"}$$

b) the only orbits without asymptotes are bound orbits — $\operatorname{Ran}\Omega_+ = \operatorname{Ran}\Omega_- =$ space $\perp$ to eigenstates of H

Asymptotic Completeness

(Difficult to prove)

True for e.g. $V \in L^3(\mathbb{R}^3)$ - see Reed + Simon, Scatt. Theory

We can easily prove a much weaker result:

Claim: $\left.\begin{matrix}\operatorname{Ran}\Omega_+\\ \operatorname{Ran}\Omega_-\end{matrix}\right\} \perp \mathcal{B} =$ boundstates (eigenstates of H)

Proof Suppose $U(t)\varphi \to U^0(t)\varphi_{in}$ as $t \to \pm\infty$

$$H\psi = E\psi$$

$$(\psi,\varphi) = (U(t)\psi, U(t)\varphi) = e^{iEt}(\psi, U^0(t)\varphi_{in})$$

But this $\to 0$ as $t \to \infty$ by the "spreading of the wave packet" argument.

$$\int d^3x\, \psi^* \varphi^0(t) \le \int d^3x\, |\psi| \frac{1}{t^{3/2}} \to 0 \text{ if } \int d^3x |\psi| \text{ exists}$$

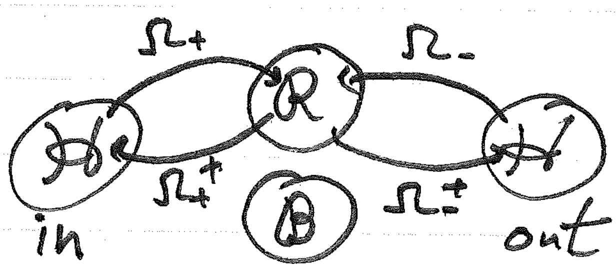
(φ_{in} gaussian)

(ψ stays localized while φ spreads out)

(Approximate arbitrary φ_{in} with finite sum of Gaussians.)

can be extended to ψ square integrable (problem arises only because of tail of ψ)

If we tried our existence proof for $\Omega^{\pm}$ on $\lim_{t\to\pm\infty} U^0(t)^\dagger U(t)\psi$, it would fail if $U(t)$ has eigenstates.
It works for $\Omega^{\pm}$ because U^0 has no eigenstates, and so makes all states spread.



B. The S-Matrix

Our goal in scattering theory is to relate in and out asymptotes. This we can now do, because

$$\psi = \Omega_+ \psi_{in} \qquad \Omega_+^\dagger \Omega_+ = \mathbb{1}$$
$$\psi = \Omega_- \psi_{out} \qquad \Omega_-^\dagger \Omega_- = \mathbb{1}$$

Hence

$$\psi_{out} = \Omega_-^\dagger \psi = \Omega_-^\dagger \Omega_+ \psi_{in}$$

or

$$\boxed{\psi_{out} = S\,\psi_{in} \quad \text{where } S = \Omega_-^\dagger \Omega_+}$$

S is the "S-Matrix", or "Scattering Operator"

The S matrix contains all information of experimental interest about scattering phenomena. In fact, we will find that, through the magic of analytic continuation, it contains all the information about bound states as well!

If Ω_+ and Ω_- have the same range (Asymptotic completeness) then $\underline{S \text{ is unitary}}$, because it is a product of unitary operators:

$$\Omega_+ : \mathcal{H} \to \mathcal{R}$$
$$\Omega_-^{+} : \mathcal{R} \to \mathcal{H}$$

Conservation of Probability:
= "What goes in, must come out"

Energy Conservation

Since S takes in asymptotes to out asymptotes, it should commute with the unperturbed energy

To show this, we first prove

$$\boxed{H\Omega_\pm = \Omega_\pm H^0} \text{ — intertwining relation}$$

$$e^{iH\tau}\Omega = \lim_{t\to\pm\infty} e^{iH\tau} e^{iHt} e^{-iH^0 t}$$
$$= \lim e^{iH(\tau+t)} e^{-iH^0 t}$$
$$= \lim e^{iH(t)} e^{-iH^0(t-\tau)}$$
$$= \lim e^{iHt} e^{-iH^0 t} e^{iH^0\tau} = \Omega e^{iH^0\tau}$$

differentiate:

$$e^{iH\tau} H\Omega = \Omega H_0 e^{iH^0\tau} \Rightarrow H\Omega_\pm = \Omega_\pm H_0$$

Also, because $\Omega_\pm^+ \Omega_\pm = 1$, we may write

$$\Omega_\pm^+ H \Omega_\pm = H_0$$

another way to see that $\Omega_\pm$ cannot be unitary unless H has no bound states (H and H_0 would have the same spectrum)

The action of H on $\mathcal{R}$ (scattering states) is unitarily equivalent to H_0!

Now it follows that S commutes with H^0

$$SH^0 = \Omega_-^+ \Omega_+ H^0 = \Omega_-^+ H \Omega_+ = H^0 \Omega_-^+ \Omega_+ = H^0 S$$

$$\Rightarrow [S, H^0] = 0$$

Since S and H^0 commute, they can, in a sense, be simultaneously "diagonalized". of course $H^0 = \frac{1}{2}p^2$ has no eigenstates

But unitary operators, like self-adjoint operators, have spectral representations

$$S = \int_{\mathbb{R}} e^{is}\, dP_s$$

$$H^0 = \int_{\mathbb{R}} E\, dP_E$$

When we say S and H^0 can be simultaneously diagonalized, we mean that each preserves the ranges of the projection-valued measures of the other

e.g. $[S, H^0] = 0 \Rightarrow [S, P_\Omega^{H_0}] = 0$ for $\Omega = [E, E + \Delta E]$

and $\quad P_\Omega^{H_0}(S P_\Omega^{H_0} \psi) = S(P_\Omega^{H_0} \psi)$

It is convenient to use the "momentum representation" in which

$$\tilde{\psi}_{out}(\vec{p}') = \int d^3_p \, \langle \vec{p}' | S | \vec{p} \rangle \, \tilde{\psi}_{in}(\vec{p})$$

$\langle \vec{p}' | S | \vec{p} \rangle$ - the matrix element of S between "improper" eigenstates of $\vec{P}$ is well defined, although the eigenstates themselves are not.

The "continuum normalization"

$\langle \vec{p}' | \vec{p} \rangle = \delta^3(\vec{p}-\vec{p}')$ is just a perverse restatement of the Fourier integral theorem (which holds for all L^2 functions):

$$\psi(\vec{x}) = \int \frac{d^3p}{(2\pi)^3}\, e^{i\vec{p}\cdot\vec{x}}\, \tilde{\psi}(\vec{p})$$

$$\text{where} \quad \tilde{\psi}(p) = \int d^3x\, e^{-i\vec{p}\cdot\vec{x}}\, \psi(\vec{x})$$

$$\langle \vec{x} | \vec{p} \rangle = \frac{e^{i\vec{p}\vec{x}}}{(2\pi)^{3/2}} \qquad \langle \vec{p}' | p \rangle = \int \frac{d^3x}{(2\pi)^3}\, e^{i(\vec{p}-\vec{p}')\cdot\vec{x}}$$

is not a function, but a distribution, it makes sense only when integrated against an L^2 function

Formally

$$\tilde{\psi}(p) = \int d^3x\, e^{-i\vec{p}\cdot\vec{x}} \int \frac{d^3p'}{(2\pi)^3}\, e^{i\vec{p}'\cdot\vec{x}}\, \tilde{\psi}(\vec{p}')$$

Illicit interchange of integration order

$$\Rightarrow \quad \tilde{\psi}(p) = \int d^3p' \left[\int \frac{d^3x}{(2\pi)^3}\, e^{i(\vec{p}'-\vec{p})\cdot\vec{x}} \right] \tilde{\psi}(\vec{p}')$$

$$= \int d^3p'\; \delta^3(\vec{p}'-\vec{p})\, \psi(\vec{p}')$$

The δ function makes sense as a representation of an operator if we remember that it must be integrated against an L^2 function

Because S commutes with H^0, we may write

$$\langle \vec{p}' | S | \vec{p} \rangle = \delta^3(\vec{p}-\vec{p}') - 2\pi i\, \delta(E_{p'}-E_p)\, t(\vec{p}',\vec{p})$$
$$= \delta^3(\vec{p}-\vec{p}') + \frac{i}{2\pi}\, \delta(E_{p'}-E_p)\, f(\vec{p}',\vec{p})$$

δ^3 is just a representation of the operator $\mathbb{1}$. (Amplitude for no scattering)

These definitions of t and f are convenient because

t, the "(on-shell) T-matrix" arises naturally in the time-independent formalism.

f, the "scattering amplitude", is closely related to the (experimentally observable) cross-section

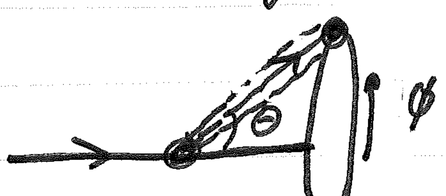
C. The Cross Section

S-matrix elements are probability amplitudes — i.e. $|(\varphi, S\psi)|^2$ represents the probability that a state asymptotic to ψ in the distant past evolves into a state asymptotic to φ in the distant future.

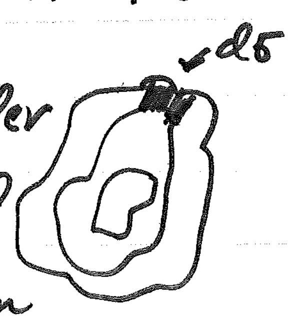
How is S related to what is actually measured in a scattering experiment?

Classical Particle Scattering

In classical mechanics, we can define scattering angles (θ, ϕ) for an orbit w/ straight line asymptotes.



For such orbits, consider a small solid angle $d\Omega = \sin\theta\, d\theta\, d\phi$ centered at (θ, ϕ). The orbits which fill this solid angle pierce the "impact parameter" plane in a region of area $d\sigma$



The differential cross section is defined as $\frac{d\sigma}{d\Omega}(\theta,\phi)$

If we imagine filling the "impact parameter plane" with a homogeneous beam with

Φ = particles/area

and

$N(d\Omega)$ = no. of particles scattered into $d\Omega$,

then $N(d\Omega) = \frac{d\sigma}{d\Omega}\ \Phi$

Quantum Mechanics

To define a scattering angle in quantum mechanics, we must work with momentum "eigenstates" $|\vec{p}\rangle$, which specify a direction in space.

As we have seen, we can make sense of these eigenstates by regarding

$$d^3p\,|\psi_{in}(\vec{p})|^2$$
$$d^3p\,|\psi_{out}(\vec{p})|^2$$

as probability distributions in momentum space

We wish to consider $\psi_{in}(\vec{p})$ a narrow wave packet in momentum space. (In practice, this means that $\psi_{in}(\vec{x})$ is broad in position space compared to characteristic "width" of the potential $V(\vec{x})$.) We wish to calculate probability that a measurement of the momentum of ψ_{out} gives a value in some small interval $[p', p'+dp']$. We might as well work with "momentum eigenstates", as long as we realize that we are calculating a probability distribution for wave packet states, as described above.

A convenient way to carry out the limiting procedure implied by the use of momentum eigenstates is to put the world in a box with periodic boundary conditions. (This derivation is a bit heuristic.)

Consider a cubical box of size a, volume $V = a^3$. The momentum operator has eigenstates

$$\langle \vec{x} | \vec{p} \rangle^a = \frac{1}{\sqrt{V}} e^{i \vec{p} \cdot \vec{x}} \qquad \vec{p} = \frac{2\pi}{a}(n_x, n_y, n_z)$$

(with the conventional discrete normalization

$$\langle \vec{p}' | \vec{p} \rangle = \delta_{n_x n_x'} \delta_{n_y n_y'} \delta_{n_z n_z'} \text{)}$$

If the world is in a box, the S-matrix does not exist. That is, we cannot define asymptotic states.

Instead let us define $S_T = e^{iH_0 \frac{T}{2}} e^{-iH\frac{T}{2}} e^{-iH\frac{T}{2}} e^{+iH_0\frac{T}{2}}$

without taking $T \to \infty$

We intend to take $T \to \infty$ limit as we let $V \to \infty$

Now, consider scattering in the nonforward direction, $\vec{p} \neq \vec{p}'$ (We can't define cross section for $\vec{p} = \vec{p}'$, except as a limit)

$$^a\langle \vec{p}' | S_T - 1 | \vec{p} \rangle^a = \frac{i}{2\pi} \frac{(2\pi)^3}{V} \delta_T(E_p' - E_p) f^{VT}(\vec{p}', \vec{p})$$

Here $\frac{(2\pi)^3}{V}$ is a normalization factor, inserted so $f^{VT} \to f$ as $V, T \to \infty$

δ_T is an approximation to a δ function with a width of order $1/T$

$$\left[\delta_T(E - E') = \frac{1}{2\pi} \int_{-T/2}^{T/2} dt\, e^{i(E-E')t} = \frac{1}{\pi} \frac{\sin(E-E')\frac{T}{2}}{E - E'} \right]$$

Transition probability is

$$P_{\vec{p}',\vec{p}} = \frac{1}{(2\pi)^2}\left(\frac{(2\pi)^3}{V}\right)^2 |\delta_T(E_{p'}-E_p)|^2 \, |f^{VT}(\vec{p}',\vec{p})|^2$$

and, as $T\to\infty$, $\delta_T^{\,2} \to \frac{T}{2\pi}\delta(E_p'-E_p)$

and $\delta(\frac{1}{2}p'^2 - \frac{1}{2}p^2) = \frac{1}{p}\delta(p'-p)$

Hence we have

$$P_{\vec{p}',\vec{p}} = \frac{(2\pi)^3}{V^2} T \frac{1}{p}\delta(p-p')|f^{VT}|^2$$

To convert this to a continuum probability distribution, we recall that the density of states in momentum space is

$$dN = \frac{V}{(2\pi)^3}d^3p = \frac{V}{(2\pi)^3}p^2 dp\, d\Omega$$

So the probability of a transition to a state in solid angle $d\Omega$ is

$$\int dp'\, P_{\vec{p}',\vec{p}} = \frac{T}{V}\frac{1}{p}|f^{VT}|^2 p^2 d\Omega$$

$\Rightarrow$ transition rate $= \frac{p}{V}|f^{VT}|^2 d\Omega$

Finally, to find the cross section, we must divide by the "incident flux" associated with the state $|\vec{p}\rangle^a$

It has probability density $\frac{1}{V}$ and velocity p

$\Rightarrow$ Flux $\frac{p}{V}$, and differential cross section is

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\vec{p}',\vec{p})|^2}$$

In our scattering experiment, we measure only the absolute value of the scattering amplitude.

D. The Optical Theorem

The unitarity of $S \Rightarrow$ a condition on f.

Define R by $\quad S = 1 + R$

Then $\quad S^{+}S = 1 = (1+R)^{+}(1+R) = 1 + R + R^{+} + R^{+}R$

$$R + R^{+} = -R^{+}R$$

or, in the momentum representation,

$$\langle \vec{p}\,'|R|\vec{p}\rangle + \langle \vec{p}\,'|R^{+}|\vec{p}\rangle = -\int d^3p''\langle \vec{p}\,'|R^{+}|\vec{p}\,''\rangle\langle \vec{p}\,''|R\,|\vec{p}\rangle.$$

Now, recall $\quad R = \frac{i}{2\pi}\delta(E_{p'} - E_p)\, f(\vec{p}\,';\vec{p})$

$\Rightarrow$ (factoring out a δ function)

$$f(\vec{p}\,';\vec{p}) - f(\vec{p},\vec{p}\,')^{*} = \frac{i}{2\pi}\int d^3p''\,\delta(E_{p''} - E_p)\, f(\vec{p}\,'';\vec{p}\,')^{*} f(\vec{p}\,'';p)$$

and $\quad \delta(E_{p''} - E_p) = \frac{1}{p}\delta(p - p'')$

or
$$\boxed{f(\vec{p}\,';\vec{p}) - f(\vec{p},\vec{p}\,')^{*} = \frac{i}{2\pi}p\int d\Omega\, f(\vec{p}\,'',\vec{p}\,')^{*} f(\vec{p}\,'';\vec{p})}$$

Generalized Optical Theorem

Now, consider the special case $\vec{p} = \vec{p}\,'$

$$2i\,\mathrm{Im}\, f(\vec{p},\vec{p}) = \frac{i}{2\pi}p\int d\Omega\, |f(\vec{p}\,'';\vec{p})|^2$$

This integral is $\quad \int d\Omega\, \frac{d\sigma}{d\Omega} = \sigma(\vec{p}) \quad$ The total cross-section

We have

$$\boxed{\mathrm{Im}\, f(\vec{p},\vec{p}) = \frac{p}{4\pi}\sigma(\vec{p})}$$

Optical Theorem

- The optical theorem relates the imaginary part of the forward scattering amplitude to the total cross section - it is a consequence of unitarity alone.
- We recall that f is defined by subtracting $\mathbb{1}$ from S - so forward scattering means the limit of f as $(\theta, \phi) \to 0$.
- The "optical theorem" is named after the corresponding result in EM scattering which relates the imaginary part of the index of refraction of a medium to the absorption cross section - there too it merely expresses conservation of probability.

III. Analytic Functions

We have reduced the problem of analyzing the scattering behavior of a system to calculation of the S-Matrix. We need to develop tools which will allow us to do such computations.

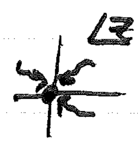
Calculations are usually done using, not the time-dependent formalism we have developed, but a time-independent formalism

Before developing the time-independent formalism, we will review some mathematics, which we will be applying throughout this course.

A. The Derivative

Consider $f: \mathbb{C} \to \mathbb{C}$

Define $f'(z) = \lim\limits_{\Delta z \to 0} \dfrac{f(z+\Delta z) - f(z)}{\Delta z}$



For limit to exist, it is required that it be the same as Δz approaches 0 along <u>any direction</u> in the z plane

<u>Cauchy-Riemann conditions:</u>

Let $f = u + iv$ $\quad z = x + iy$ $\quad u, v, x, y$ real

$f'(z)$ exists $\Rightarrow$

$$\frac{\partial f}{\partial x} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = \frac{\partial f}{\partial (iy)} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}$$

$$\Longrightarrow \boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}}$$

These conditions are also sufficient:

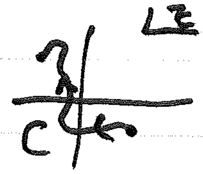
$$\Delta f = \frac{\partial u}{\partial x}\Delta x + \frac{\partial u}{\partial y}\Delta y + i\left(\frac{\partial v}{\partial x}\Delta x + \frac{\partial v}{\partial y}\Delta y\right)$$

C-R conditions $\Rightarrow$ $= \frac{\partial u}{\partial x}(\Delta x + i\Delta y) + i\frac{\partial v}{\partial x}(\Delta x + i\Delta y)$

$$= \left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right)\Delta z$$

We say f is *analytic* at z if $f'(z)$ exists in a neighborhood of z

B. Integrals



contour integral

$$\int_C f(z)\,dz = \int_C (u\,dx - v\,dy) + i\int_C (u\,dy + v\,dx)$$

Suppose C is a closed curve

Green's Theorem $\Rightarrow$ $\int_C f(z)\,dz = \int_{\text{Area}} dx\,dy\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + i\int_{\text{Area}} dx\,dy\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)$

(Traced counterclockwise)

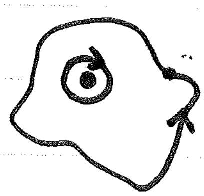
$= 0$ by Cauchy-Riemann conditions

To prove this, it is not necessary to assume f' is continuous

i.e. $\boxed{\int_C f(z)\,dz = 0}$ if C is the boundary of a region of analyticity of f (and f is analytic on C)

Cauchy Theorem

Cauchy integral formula:



f analytic on and inside C and z inside C $\Rightarrow$ $\frac{f(z')}{z'-z}$ also analytic except at z.

Cauchy Theorem $\Rightarrow$

$$\frac{1}{2\pi i}\int_C \frac{f(z')}{z'-z}\,dz' = \frac{1}{2\pi i}\int_{C'} \frac{f(z')}{z'-z}\,dz'$$

we can "shrink" C to small circle around z

$$z'-z = Re^{i\theta} \qquad dz' = i\,Re^{i\theta}d\theta$$

$$\Rightarrow \frac{1}{2\pi i} f(z)\int_0^{2\pi} i\,d\theta = f(z)$$

i.e. $\boxed{f(z) = \frac{1}{2\pi i}\int_C dz' \frac{f(z')}{z'-z}}$

counterclockwise sense

A central result of the theory of analytic functions

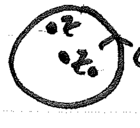
C. Power Series

A remarkable property of analytic functions is:
The derivative of an analytic function is analytic.
i.e. analytic functions have derivatives <u>of all orders</u>!

This can be established by "differentiating under the integral sign" in the Cauchy formula, which can easily be shown to be justified.

$$f^{(n)}(z) = \frac{n!}{2\pi i}\int_C dz' \frac{f(z')}{(z'-z)^{n+1}}$$

- To expand $f(z)$ in power series, suppose f analytic in a circle about z_0

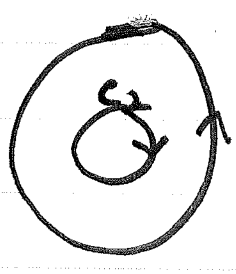


C

$$f(z) = \frac{1}{2\pi i}\int dz' \frac{f(z')}{z'-z} \qquad \frac{1}{z'-z} = \frac{1}{z'-z_0-(z-z_0)} = \frac{1}{z'-z_0}\sum\left(\frac{z-z_0}{z'-z_0}\right)^n$$

$$\Rightarrow f(z) = \frac{\sum_n}{2\pi i}\int dz' f(z')\frac{(z-z_0)^n}{(z'-z_0)^n} = \sum_n \frac{f^n(z_0)}{n!}(z-z_0)^n$$

This series is uniformly convergent inside the circle.



C_1

- For a function analytic between concentric circles

$$f(z) = \frac{1}{2\pi i}\int_{C_1} dz' \frac{f(z')}{z'-z} + \frac{1}{2\pi i}\int_{C_2} dz' \frac{f(z')}{z'-z}$$

expand in powers of $\frac{z-z_0}{z'-z_0}$ expand in powers of $\frac{z'-z_0}{z-z_0}$

$$\Rightarrow f(z) = \sum_n a_n(z-z_0)^n + \sum b_n \frac{1}{(z-z_0)^n}$$

$$b_n = \frac{1}{2\pi i}\int_{C_2} f(z')\,dz'(z'-z_0)^{n-1}$$

- If an analytic function has a zero, <u>the zero is isolated</u> (there is a neighborhood in which it is the only zero)

if $f(z)\not\equiv 0$, $\quad f(z) \sim (z-z_0)^m \,\underbrace{[a_m + a_{m+1}(z-z_0) + \cdots]}_{\text{has no zero in neighborhood of } z_0}$

D. Residue Theorem

If f is analytic in neighborhood containing z_0, except at z_0 (isolated singular point), then f has Laurent series expansion

- If series terminates $\sum_{n=1}^{N} \frac{b_n}{(z-z_0)^n}$ + analytic

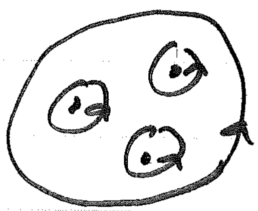
  z_0 is a pole

- If series contains infinite number of terms, essential singularity

$$\frac{1}{2\pi i}\int_C dz\, f(z) = b_1$$

" = Residue of the function f at the isolated singular point z_0"

Hence, if f is analytic in region bounded by C, except for isolated singular points, then



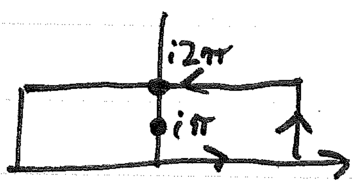
$$\boxed{\int_C f(z) = 2\pi i \sum_n R_n}$$

R_n ← residue at singular point n

Residue Theorem

We can use the residue theorem to calculate many definite integrals

Example: $I = \int_{-\infty}^{\infty} \frac{e^{ax}}{1+e^x}dx \qquad 0<a<1$



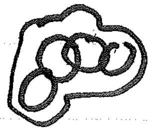
$$2\pi i\left(-e^{i\pi a}\right) = \int_{-\infty}^{\infty} dx\, \frac{e^{ax}}{1+e^x} - \int_{-\infty}^{\infty} dx\, \frac{e^{a(x+2\pi i)}}{1+e^x}$$

$$= \left(1-e^{2\pi i a}\right) I$$

$$\Rightarrow I = -2\pi i \frac{e^{i\pi a}}{1-e^{2\pi i a}} = \pi \frac{1}{\left(e^{i\pi a}-e^{-i\pi a}\right)/2i} = \frac{\pi}{\sin \pi a}$$

You will do other examples on the homework.

E. Analytic Continuation



If f has zeros with a limit point at z_0 then $f=0$ in a neighborhood of z_0, because $f=0$ is the only analytic function w/ zeros which are not isolated.

But then $f=0$ throughout its domain of analyticity (if connected), because f has a convergent power series with a finite radius of convergence about every point in its domain of analyticity – and we can fill the domain with intersecting circles

This is the basis of <u>analytic</u> <u>continuation</u>

If two functions are equal on a set which has a limit point, then they are equal on their common domain of analyticity

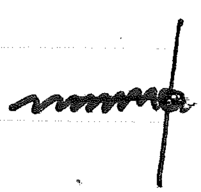
E.g. f is determined <u>uniquely</u> in region by its value along an arc!!

F. Branch Cuts and Riemann Surfaces

Some functions are locally analytic, but are <u>multivalued</u>.

E.g. $\quad f(z) = z^{1/n} \qquad z = Re^{i\Theta} \Rightarrow$

$$f = R^{1/n} e^{i(\Theta + 2\pi k)/n}$$

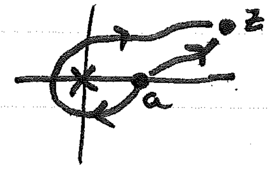


This function has n <u>branches</u>, a <u>branch point</u> at $z=0$ and a <u>branch cut</u>, which we may choose to be along negative real axis, across which it is discontinuous. We can represent f as a function on a twisting <u>Riemann surface</u>, on which it is single-valued, and singular only at the branch point.

$$F(z) = \log z = \ln R + i\Theta$$

The branch <u>cut</u> is an artifice, but the branch <u>point</u> is a genuine singularity which cannot be removed.

E.g.



consider the function

$$g(z) = \int_a^z dz' \, \frac{f(z')}{z'}$$

where $f(z')$ is analytic throughout the complex plane (entire).

$g(z)$ is <u>infinite-valued</u>, because the contour from a to z can wind around the pole at $z=0$ an arbitrary number of times. g has a branch <u>point</u> at $z=0$. (Integration takes <u>poles</u> to branch points.)

The discontinuity across the <u>cut</u> separating "first sheet" from second sheet" is $2\pi i f(0)$.

$= \text{disc}\, g(x)$

$= g(x+i\epsilon) - g(x-i\epsilon)$

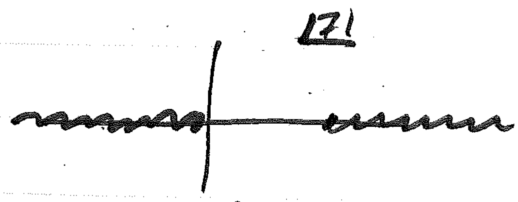
- <u>Reflection</u> <u>Principle</u>

A real valued function $f(x)$ on an interval of $\mathbb{R}$ has a unique analytic continuation throughout $\mathbb{C}$. This continuation obeys

$$\boxed{f(z^*) = f(z)^*} \quad \text{Reflection Principle}$$

This is obvious, because power series coefficients are real. To prove it, it suffices to observe that

$f(z^*)^*$ is analytic if $f(z)$ is (satisfies C-R conditions), and is equal to $f(z)$ on real interval. Thus $f(z) = f(z^*)^*$ throughout domain of analyticity, because analytic continuation is <u>unique</u>



For such a function, the discontinuity across a cut on the real axis is imaginary:

$$\text{Disc} f = f(x+i\epsilon) - f(x-i\epsilon) = f(x+i\epsilon) - f(x+i\epsilon)^*$$
$$= 2i \, \text{Im}\, f(x+i\epsilon)$$

(Clearly true for $\log z$ and $z^{1/n}$ (on the $k=0$ branch))