Review of Quantum Mechanics, cont.

1 Expansion of a plane wave in spherical harmonics

We want to develop solutions for scattering problems. In a scattering problem we usually have a beam of particles moving in some direction toward a scattering center. This defines a coordinate axis to be taken as z in a Cartesian frame. However scattering is normally solved in spherical coordinates with the scattering center at the coordinate origin. Thus we need to transform a plane wave into the spherical coordinate system. The plane wave solution to the Schrodinger equation is then written, e^{ikz} with a normalization of 1. Use the completeness of the spherical harmonics to write;

$$e^{i\vec{k}\cdot\vec{r}} = e^{iprcos(\theta)} = \sum C_n Y_l^0$$

and by orthorgonality of the Y_n^m

$$C_n = 2\pi \int_0^\pi \sin(\theta)\, d\theta\, Y_n\, e^{ikr\cos(\theta)}$$

Substitute $Y_n^0 = \sqrt{\frac{2l+1}{4\pi}}\, P_n$ and the integral representation for the spherical Bessel function, $j_n(kr) = \frac{-i^n}{2} \int_0^\pi \sin(\theta)\, d\theta\, e^{ikr\cos(\theta)}\, P_n(\cos(\theta))$ we obtain

$$e^{i\,\vec{k}\cdot\vec{r}} = 4\pi \sum_l i^l\, [4\pi(2l+1)]^{1/2}\, j_l(kr)\, Y_l^0$$

Use the addition theorem to write this in arbitrary coordinate frames;

$$e^{i\,\vec{k}\cdot\vec{r}} = 4\pi \sum_{l,m} i^l\, j_l(kr)\, Y_l^m(\hat{k})\, Y_l^{m\,*}(\hat{r})$$

2 Scattering

The propagation of a wave packet in space is a superposition of particle waves of a number of frequencies. We look at one frequency component, assuming that we can construct a wave packet as needed. The scattering problem assumes that the wave packet (particle) moves freely at a distance far from a scattering center, both before and after scattering. Only near the scattering center does the particle interact, which causes the scattering. Write Schrodinger equation as;

$$E \,=\, p^2/2m \,+\, V(\vec{r}) \,+ U(\vec{r})$$

where $U \,\rightarrow\, 0$ as $|\vec{r}| \rightarrow \infty$. Here U is the potential that causes the scattering, and we take V to vanish to simplify the exposition. The wave function solution for large r will have the form;

$$\psi \,\rightarrow\, A\, e^{ikz}$$

That is, this is a plane wave with wave number $k \,=\, p/\hbar$ (the frequency $\omega \,=\, p^2/2m\hbar$ and time are suppressed in this notation) moving in the z direction. The multiplying constant A provides the normalization. Near, but outside, the scattering center, there should be outgoing spherical waves having a radial form, e^{ikr}/r, and an angular dependence which we express by the function, $f(\theta, \phi)$. Thus we write;

$$\psi_{r \rightarrow \infty}\, A[e^{ikz} \,+\, f(\theta, \phi)\, \frac{e^{ikr}}{r}]$$

It is interesting to note that in the very forward direction there will be an interference between the incident and scattered waves. This is the Ramsauer-Townsend effect which is the diffraction of the scattered particle as it moves through and around the scattering center. At sufficiently large angles only the scattered wave is considered. (Although mathematically the plane wave is treated as infinite in extent ina the directions perpendicular to the beam, z. In reality the wave is only large compared to the transverse dimensions of the scattering center).

The incident flux which is equal to the number of incident particles per cross sectional area of the scattering center is given by the probability density times the velocity.

$$\frac{\hbar}{2im}\, [\psi^*\, \vec{\nabla}\psi \,-\, \vec{\nabla}\psi^*\, \psi] \cdot \vec{V_g} \,=\, V_g|A|^2$$

The scattered flux is obtained in the same way, and evalusted to be;

$$V|A|^2 \frac{|f|^2}{r^2}$$

The cross section for the scattering is defined as the number scattered per unit time into the area subtended by a solid angle $d\Omega$ per incident flux. This is written;

$$d\sigma \,=\, [V|A|^2 \frac{|f|^2}{r^2}]\, \frac{r^2\, d\omega}{|A|^2\, V}$$

Resulting in the expression

$$\frac{d\sigma}{d\Omega} \,=\, |f(\theta, \phi)|^2$$

It is clear that the normalization A is unimportant as the number scattered particles scales linearly with the number of incident particles, and A cancels out of the cross section.

Now return to the Schrodinger equation for a 3-D spherically symmetric potential and find the radial solution in the form, $F(r)$.

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} + [U(r) + \frac{l(l+1)\hbar^2}{2mr^2}]\chi = E\chi$$

where $F(r) = \chi/r$. The most general form for F for a specific value of l is a superposition of spherical Bessel functions.

$$F_l = A_l[cos(\delta_l)\, j_l(kr) - sin(\delta_l)\, \eta_j(kr)]$$

with j_j and η_l the spherical Bessel and Hankel functions, respectively. The constant δ_l is a real phase and A is a complex normalization. We use the limiting values of the Bessel functions as $r \rightarrow \infty$ to write;

$$F_{l\, r\rightarrow\infty} = A_l \frac{\sin(kr - l\pi/2 + \delta_l)}{kr}$$

Now substitute the expansion of a plane wave in spherical coordinates into the asymptotic solution and equate the equations

$$e^{ikr\cos(\theta)} = \sum_{l=0}^{\infty} (2l+1)\, i^l\, j_l(kr)\, P_l(\cos(\theta))$$

After a little algebra;

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)\, (e^{2i\delta_l} - 1)\, P_l(\cos(\theta))$$

The differential cross section is;

$$\frac{d\sigma}{d\omega} = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1)\, (e^{2i\delta_l} - 1)\, P_l(\cos(\theta)) \right|^2$$

And the total cross section

$$\sigma_T = 2\pi \int_0^{\pi} \sin(\theta)\, d\theta \frac{d\sigma}{d\omega}$$

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l)$$

Now the total cross section can be related to $f(\theta = 0)$ by using $P_l(1) = 1$ for all l. Thus

$$f(0) = \frac{1}{2ik} \sum_{l=o}^{\infty} (2l+1)(e^{2i\delta_l} - 1)$$

which gives;

$$\sigma = \frac{4\pi}{k} Im[f(0)]$$

The value of the constant δ_l is the phase shift for a given partial wave (value of l). Remember from the treatment of the transmission problem we expect a shift in phase between the incident and outgoing waves. A repulsive potential generally gives a negative phase shift and an attractive potential gives a positive phase shift.

As an example, consider scattering by a black sphere (completely absorbing sphere of radius $r = a$. In this case we take $U(r) = \infty$ for $r > a$ and $U(r) = 0$ for $r < a$. One can solve the Schrodinger equation for $R > a$ as an outgoing spherical wave which must vanish at $r = a$. This results in $tan(\delta_l) = fracj_l(ka)neta_l(ka)$ and when $k = 0$ the total cross section becomes;

$$\sigma_T = 4\pi a^2$$

or 4 times its classical value of πa^2

3 Mechanical example of resonance

Excited particle states, at high energy in particular, are not stable. However they can still be recognized as states if they exhibit resonant structure. We look at a simple mechanical model of resonance to understand the physics. The mechanical model is illustrated in the simple cartoon in Figure 1. In this figure a mass, M, is driven away from equilibrum, x_0 by a harmonic force, F. The mass has a restoring force applied by a spring of spring constant, k, and there is a resistive force proportional to the velocity. The equation of motion given by Newton's laws is;

$$M\frac{d^2x}{dt^2} + R\frac{dx}{dt} + kx = F_0 \sin(\omega t)$$

We choose to look for a steady state solution of the form, $x = A\sin(\omega t + \phi)$. The constant ϕ is a phase factor to be determined. Substitute this into the differential equation to obtain the algebraic equation;

$$-M\omega^2 A \sin(\omega + \phi) + R\omega \cos(\omega t + \phi) + kA \sin(\omega t + \phi) = F_0 \sin(\omega t)$$

Use trig identities to separate the harmonic forms, and then collect terms in $\sin(\omega t)$ and $\cos(\omega t)$

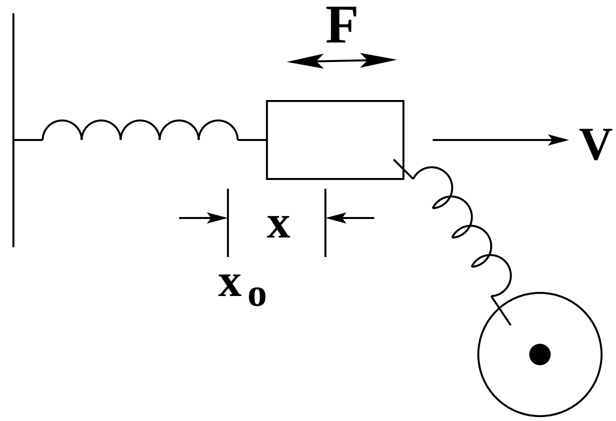

Figure 1: A mechanical system to investigate resonance

$$\tan(\phi) \;=\; \frac{R\omega}{M\omega^2 - k}$$

$$A \;=\; \frac{F_0/M}{[(\omega^2 - \omega_0^0)^2 \;+\; (R/M)^2\omega^2]^{1/2}}$$

Here $\omega_0 \;=\; k/M$ and sometimes $\Gamma^2 \;=\; (R/M)^2$. Note that as $\omega \to \omega_0$ the oscillation amplitude increases. Indeed as $R \to 0$ the amplitude increases to ∞. The maximum amplitude is obtained from $\frac{dA}{d\omega} \;=\; 0$. At the value of maximum amplitude;

$$\omega_{max} \;=\; \sqrt{kM - (1/2)(R/M)^2}$$

At this value of ω

$$A \;=\; \frac{F_0}{(R/M)[Mk - R^2/2]^{1/2}}$$

This is the resonance condition. The sharpness of the resonance peak is called the Q of the system. Obviously as $R \to 0$ the amplitude becomes infinite and the width decreases to zero. Now look at the power that is put into the system, $P \;=\; \vec{F} \cdot \vec{V}$. This is the instantaneous work done by the driving force on the system.

$$P \;=\; \omega F_0 A[\sin(\omega t)\cos(\omega t)\cos(\phi) \;-\; \sin^2(\omega t)\sin(\phi)]$$

There is obviously power that flows into and out of the system in harmonic motion. When averaged over a period the power is the energy input to the system over the period;

$$\langle P \rangle \;=\; \frac{\omega F_0 A}{2}\sin(\phi)$$

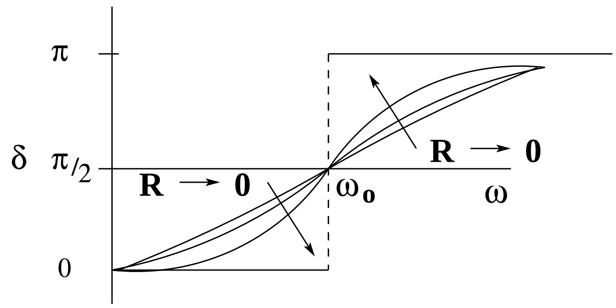

Figure 2: Phase relations for the driven oscillator

$$\sin(\phi) \;=\; \frac{R\omega}{[(M\omega^2 - k)^2 + (k\omega)^2]^{1/2}}$$

The energy lost is $[R\frac{dx}{dt}]\,dx$ and this is seen to equal the average power input from the driving force. Note that this is the energy expended in the resistance. Look at the phase difference between the amplitude and the average power when $R = 0$ Figure 2.

$$A \;=\; \frac{F_0/M}{\omega_0 - \omega^2}$$

For $\omega < \omega_0$ the amplitude is in phase with the driving force, $\phi = 0$. When $\omega > \omega_0$ the phase is π. In both cases the average power input is zero. Exactly at resonance $\omega = \omega_0$ the phase is $\pi/2$. As the resistance increases, the phase transitions between 0 and π in a continuous way passing through $\pi/2$ at resonance.

This model applies to many phenonmena in physics from mechanical motion, electrical circuits, and particle physics. For particle physics, which is the subject here, resonant states are created by collisions with other particles (Forces) that cause oscillations in the structure of the particle system. A resonant state has a maximum amplitude at a particular energy (frequency) approximating a bound wave function.

4 Relativistic wave equations

When Schrodinger proposed his non-relativistic wave equation he alos proposed a relativistic version given by the kinematic relation;

$$E^2 \;=\; p^2c \,+\, (mc^2)^2$$

The energy operator and the momentum operator are to be used as before and the energy included the rest mass. This equation is valid for a free particle without an external potential. It has a plane wave solution of the form $e^{\pm i(\vec{k}\cdot\vec{r} - \omega t)}$ which obviously satisfies the relativistic wave equation. The probability current S as previously defined also satisfies a conservation equation that is identical to the non-relativistic one. However one notes that ;

$$P(\vec{r}, t) \;=\; \frac{i\hbar}{2mc^2}\,[\psi^* \frac{\partial \psi}{\partial t} \;-\; \frac{\partial \psi^*}{\partial t}\,\psi]$$

is not positive definite. While it could be multiplied by the particle charge, e, and interpreted as a charge density, there is still an interpretation of what probabilities mean.

Obviously relativistic QM includes states of negative energy. ther is also the problem of including interactions into the equation. Consider the later problem first. If the interaction has 4-vector form, $(\phi, \vec{A})$, then it satisfies a Lorentx transformation where the scalar component acts as an energy and the vector component acts as a momentum. An example is the electromagnetic field with $e\phi$ the energy obtained from the scalar potential ϕ and $e\vec{A}$ obtained from the vector potential. In this case the relativistic equation has the form;

$$(E - \phi) \;=\; (c\vec{p} - e\vec{A})^2 \;+\; (mc^2)^2$$

Dirac attempted to address the problem of negative energy states by trying to find a wave equation linear in the energy. The simplest case assumes;

$$E \;=\; -c\vec{\alpha}\cdot\vec{p} - \beta\, mc^2$$

To find the constants, $\vec{\alpha}$ and β substitute this into the linear wave equation, $i\hbar\,\frac{\partial}{\partial t}\,\psi \;=\; E\,\psi$ and also require that $E^2 = (pc)^2 + (mc^2)^2$. This requires that these constants are 4-D matrices.

$$\beta \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\alpha_x \;=\; \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_y \;=\; \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

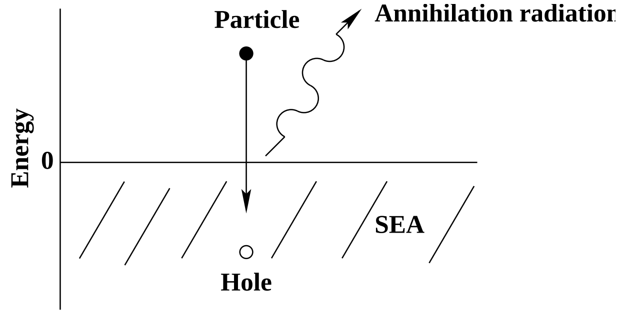

Figure 3: Interpretation of negative energy states

$$\alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

One can see the sub-matricies that depend on the Pauli spin matricies introduced earlier. The wave function is then a 4-component vector, and probability defined by $P = \psi^* \psi$ is positive definite. However this equation also introduces solutions having both positive and negative energies and a negative rest mass. the negative energy states cannot be ignored since a particle can transition from a positive energy state to a negatice energy state. Dirac proposed that the negative energy states are filled so tis transition does not occur. However, a hole in the negative energy sea is to be interpreted as an anti-particle with positive energy that travels backward in time, and has a charge equal to the negative of its positive energy counterpart, Figure 3 .

5 Lagrangian formulation

The path that a particle moves under conservative motion is that of stationary action.

$$A = \int_{t1}^{t2} dt \, \mathcal{L}[q_i(t), \dot{q}(t), t)]$$

where q and $\dot{q}$ are conjugate variables of the Lagrangian. To have a proper relativistic lagrangian we take this over into an integral over proper time $\gamma \mathcal{L}$. For the moment look at the non-relativistic action. The variation od the action yields the Euler Lagrange equations;

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} \mathcal{L} - \frac{\partial}{\partial q} \mathcal{L} = 0.$$

To proceed relativistically one introduces a relativistically invarient Lagrangian, and avries the action to get the Euler Lagrange equations.