221B Lecture Notes
Scattering Theory IV

1 Coulomb scattering

The case of Coulomb potential is somewhat special because the potential turn off at infinity rather slowly. In fact, the formalism we used so far assumed that the potential dies quickly enough to justify the asymptotic form

$$\psi(\vec{x}) \sim e^{ikz} + f(\theta)\frac{e^{ikr}}{r}. \tag{1}$$

This asymptotic behavior, however, is not valid for the Coulomb potential. Coulomb pontential is long-ranged and distorts the wave function even at large distances. In order to see this, we need to solve the equation exactly.

As usual, we go back to the Schödinger equation

$$\left[-\frac{\hbar^2}{2m}\Delta + \frac{ZZ'e^2}{r}\right]\psi(\vec{x}) = E\psi(\vec{x}). \tag{2}$$

We introduce some notations:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{1}{2}mv^2 \qquad \left(v = \frac{\hbar k}{m}\right), \tag{3}$$

$$\gamma = \frac{ZZ'e^2}{\hbar v} = \frac{1}{ka_B} \qquad \left(a_B = \frac{\hbar^2}{ZZ'e^2 m}\right). \tag{4}$$

The dimensionless parameter γ controls the impact of the Coulomb field on the wave function. In terms of these quantities, the Schrödinger equation can be written much more simply as

$$\left[\Delta + k^2 - \frac{2\gamma k}{r}\right]\psi(\vec{x}) = 0. \tag{5}$$

To solve Eq. (5), we take the ansatz

$$\psi(\vec{x}) = e^{ikz} f(u), \qquad u = r - z. \tag{6}$$

By substituting the ansatz into Eq. (5), we find

$$u\frac{d^2}{du^2}f + (1 - iku)\frac{d}{du}f - \gamma k f = 0. \tag{7}$$

Introducing yet another variable $v = iku = ik(r - z)$, it becomes

$$v \frac{d^2}{dv^2} f + (1 - v) \frac{d}{dv} f + i\gamma f = 0. \tag{8}$$

This is a differential equation of Laplace-type and hence its solution is given in terms of a confluent hypergeometric function. Putting all pieces together, the solution is given as

$$\psi(\vec{x}) = A e^{ikz} F(-i\gamma | 1 | ik(r - z)). \tag{9}$$

A is an arbitrary overall normalization factor. The exact solutions are sometimes called Coulomb harmonics.

Details of the hypergeometric functions are not of our interest. But we are interested in the asymptotic behavior of the function. By choosing the normalization factor $A = \Gamma(1 + i\gamma)e^{-\pi\gamma/2}$ for convenience, the asymptotic behavior is given as

$$\begin{aligned} \psi \quad \sim \quad & e^{i(kz + \gamma \log k(r-z))} \left[1 + \frac{\gamma^2}{ik(r-z)} + \cdots \right] \\ & - \frac{\gamma}{k(r-z)} \frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)} e^{i(kr - \gamma \log k(r-z))} \left[1 + \frac{(1+i\gamma)^2}{ik(r-z)} + \cdots \right]. \end{aligned} \tag{10}$$

The terms indicated by dots are suppressed by higher powers in $1/(r - z)$. Clearly this expression is not useful when $r = z$, *i.e.*, the extreme forward region. But as we discussed in "Scattering I," the scattering cross section does not deal with the forward region because it ignores the interference term. Therefore we will not worry about the subleading terms in $1/(r - z)$ and keep only the leading term 1 in the asymptotic expansion.

The asymptotic form of the wave function in Eq. (10) is not quite that in Eq. (1), but is similar enough to allow us to read off the scattering amplitude. We slightly modify the definition of the scattering amplitude from Eq. (1) as

$$\psi(\vec{x}) \sim e^{i(kz + \gamma \log k(r-z))} + f(\theta) \frac{e^{i(kr - \gamma \log k(r-z))}}{r}. \tag{11}$$

One can check, for example using wave packets, that this generalized definition still gives the probability of the particle to be scattered in a given solid angle. Comparing Eqs. (11) and (10), we find

$$f(\theta) = -\frac{\gamma}{k} \frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)} \frac{r}{r-z} = -\frac{\gamma}{k} \frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)} \frac{1}{2\sin^2\theta/2} \tag{12}$$

The scattering cross section is then obtained by the usual formula

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{\gamma^2}{4k^2 \sin^4 \theta/2} = \left(\frac{ZZ'e^2}{4E}\right)^2 \frac{1}{\sin^4 \theta/2}. \tag{13}$$

It is a coincidence that the Born approximation and the classical calculation both agree with this exact quantum mechanical result.

The fact that we did not have to worry about logarithmic correction in the exponents to obtain the scattering amplitude may make you wonder if the distortion of the wave function is of any physical significance. For the Rutherford scattering itself, certainly it does not matter. However, the distortion has importance consequences on other processes. One prime example is the nuclear β-decay. As is well-known, nuclear β-decay transforms one type of nucleus with $A = N_p + N_n$, $Z = N_p$ to another one with the same A but a smaller atomic number $Z - 1$ by emitting an electron e^- and anti-electron-neutrino $\bar{\nu}_e$. When the β-electron escapes the nucleus, it is subject to the binding due to the Coulomb interaction. To calculate the decay matrix element, it is important to use Coulomb harmonics rather than plane waves.

Coming back to the scattering problem, now that we have the scattering amplitude, we can look for poles. Note that the Gamma function does not have zeros, and hence we look for poles of the numerator $\Gamma(1 + i\gamma)$. The poles of $\Gamma(z)$ are located at $z = 0, -1, -2, \cdots$, or in other words $-n + 1$ for $n = 1, 2, \cdots$. Therefore the poles are at

$$1 + i\gamma = -n + 1 \tag{14}$$

Recalling the definition of γ in Eq. (4), $\gamma = 1/ka_B$, we clearly need a pure imaginary k: bound states. To be in the physical region (upper half plane $k = i\kappa$ with $\kappa > 0$) to have an exponentially damping function at large radii, and to satisfy the condition Eq. (14), we need

$$\frac{1}{\kappa a_B} = -n, \tag{15}$$

or in other words a negative $a_B = \frac{\hbar^2}{ZZ'e^2 m}$. It is possible only when $ZZ' < 0$, *i.e.* when the Coulomb potential is attractive. This is indeed what we expect. The energy levels are then obtained as

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{\hbar^2}{2ma_B^2 n^2} = -\frac{Z^2 Z'^2 e^4 m}{2\hbar^2 n^2} = -\frac{Z^2 Z'^2 \alpha^2 mc^2}{2n^2}. \tag{16}$$

This is nothing but the Bohr levels of hydrogen-like atoms as expected.

2 Two-to-two Scattering

We have discussed only the scattering of a particle by a static potential. In practice, a potential is generated by another particle, and we need to discuss two-to-two scattering problems. As long as the scattering is elastic, namely if the initial state particles and final state particles are the same, what we have done applies directly to realistic problems.

The point is just the separation of the center-of-mass motion in the two-body system. Starting from the two-particle Hamiltonian,

$$H = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V(|\vec{x}_1 - \vec{x}_2|), \tag{17}$$

we separate the center-of-mass motion by defining

$$\begin{aligned} \vec{P} &= \vec{p}_1 + \vec{p}_2, & \vec{p} &= \frac{1}{2}(\vec{p}_1 - \vec{p}_2), \\ \vec{X} &= \frac{m_1\vec{x}_1 + m_2\vec{x}_2}{m_1 + m_2}, & \vec{x} &= \vec{x}_1 - \vec{x}_2. \end{aligned} \tag{18}$$

Then the Hamiltonian becomes

$$H = \frac{\vec{P}^2}{2M} + \frac{\vec{p}^2}{2\mu} + V(|\vec{x}|), \tag{19}$$

with $M = m_1 + m_2$ and $\mu = m_1 m_2/(m_1 + m_2)$. Then the problem reduces to the potential scattering problem for a particle of mass μ.

There is, however, one interesting complication due to quantum statistics. If two particles that scatter are idential particles, such as electron-electron scattering or scattering of two idential atoms, symmetry of the wave function needs to be considered. Under the interchange of two particles $\vec{x}_1 \leftrightarrow \vec{x}_2$, $\vec{p}_1 \leftrightarrow \vec{p}_2$, the center of mass motion is not affected, but the relative coordinates change their signs $\vec{x} \leftrightarrow -\vec{x}$, $\vec{p} \leftrightarrow -\vec{p}$. If they have spins, their spins need to be interchanged at the same time.

If two particles are idential spinless bosons, say two Helium atoms (assuming ^{4}He isotopes), there is no spin degrees of freedom and the interchange of particles is simply $\vec{x} \to -\vec{x}$ in the wave function. Because they are bosons, the wave function should not change under the interchange of particles, and hence the wave function must be an even function of $\vec{x}$. Therefore the asymptotic form of the wave function Eq. (1) must be changed to

$$\psi(\vec{x}) \sim e^{ikz} + e^{-ikz} + [f(\theta) + f(\pi - \theta)] \frac{e^{ikr}}{r}. \tag{20}$$

The scattering amplitude $f(\theta)$ is calculated without the statistics in consideration, and the combination in the square bracket symmetrizes it. The differential cross section is then found to be

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2. \tag{21}$$

There is a constructive interference at $\theta = \pi/2$ which can be experimentally observed. Note that one should not integrate over the entire solid angle to obtain the total cross section because (θ, ϕ) and $(\pi - \theta, \phi + \pi)$ correspond to an identical state:

$$\sigma = \int_0^{2\pi} d\phi \int_0^1 d\cos\theta \frac{d\sigma}{d\Omega}. \tag{22}$$

For two spin 1/2 fermions, there are two possible spin wave functions, symmetric $S = 1$ and anti-symmetric $S = 0$. Therefore depending on the spin wave function, we either have a anti-symmetric or symmetric spatial wave function, respectively. In particular, the differential cross section is the same for the spinless bosons Eq. (21) for the anti-symmetric spin wave function $S = 0$, while it is

$$\frac{d\sigma}{d\Omega} = |f(\theta) - f(\pi - \theta)|^2 \tag{23}$$

for the symmetric spin wave function $S = 1$. In the latter case, the differential cross section vanishes identially at $\theta = \pi/2$. This is an interesting observation, and one can actually isolate $S = 1$ combination by studying $\theta = \pi/2$ region.

Many scattering phenomena of interest are inelastic, *i.e.*, the final state particles are not the same as the initial state particles. For instance, when an electron scatters off an atom, the final state atom may be in an excited state. Or one of the electrons bound to the atom may be kicked out from the atom. These are examples of inelastic scattering problems. We will not discuss these problems, but obviously the combination of elastic and inelastic processes will tell us a great deal about the nature of the object you study by scattering processes.

3 Time-Dependent Formulation

It is useful to connect the time-independent formulation we've discussed so far with the time-dependent formalism.

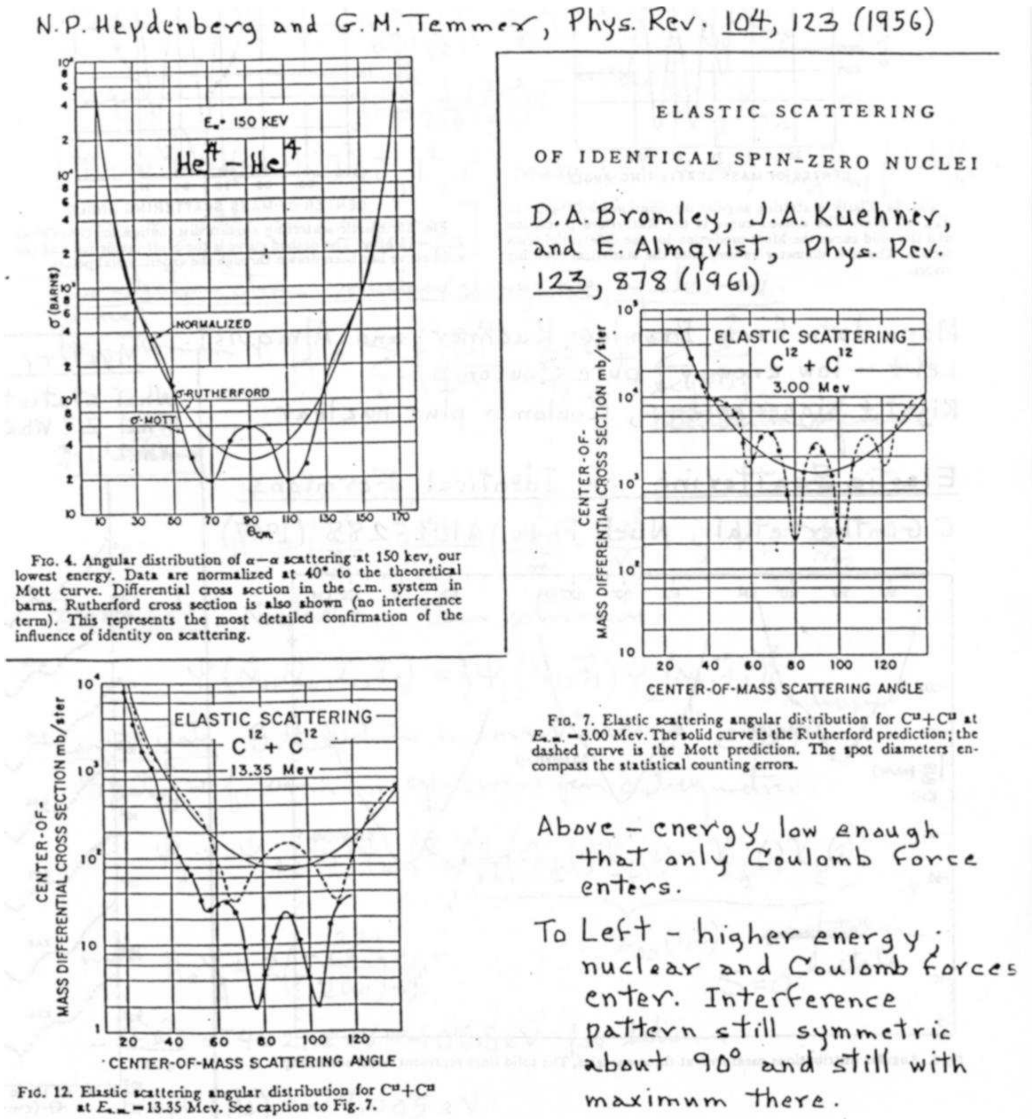

Figure 1: Data on scattering of identical particles found by Prof. Dave Jackson.

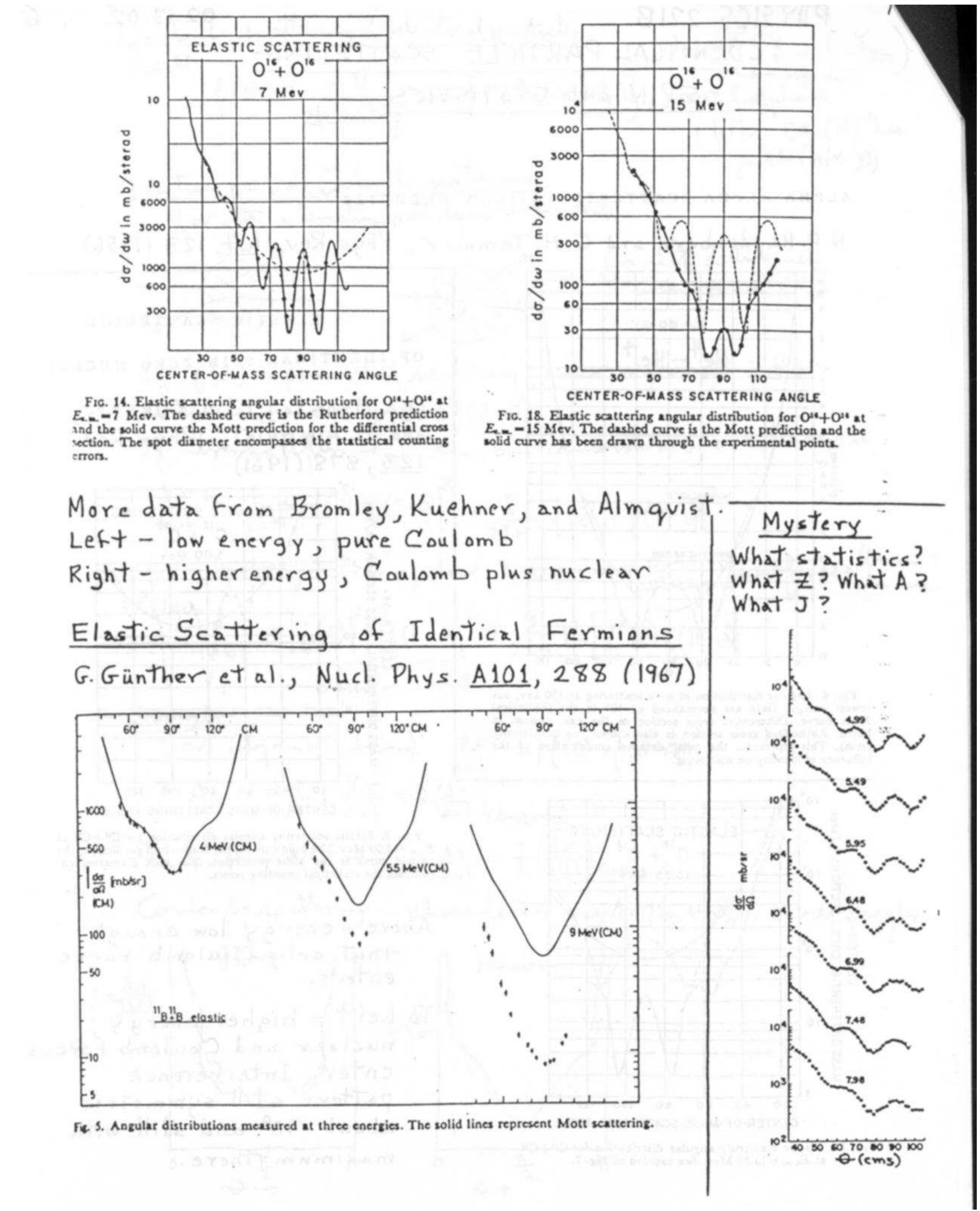

Figure 2: Data on scattering of identical particles found by Prof. Dave Jackson.

Recall the time-dependent perturbation theory from 221A. The golden-rule

$$\Gamma(i \to f) = \frac{2\pi}{\hbar}\delta(E_i - E_f)|V_{fi}|^2. \tag{24}$$

gives the rate of the initial state $|i\rangle$ to transform to the final state $|f\rangle$ to the first order in perturbation V. A "rate" is the probability per unit time.

When applied to the scattering problem, an additional issue is to define how we sum over the final states. In particular, we would like to sum over the continuum plane-wave states, and we must make the sum well-defined.

To define the sum over the continuum states, it is useful to consider the system in a cube of size L. The volume is therefore L^3. We impose the periodic boundary condition, namely that the wave function must be periodic $\psi(x,y,z) = \psi(x+L,y,z) = \psi(x,y+L,z) = \psi(x,y,z+L)$. In the limit of large L, we expect physics does not depend on the boundary condition. The plane-wave solutions in this box are given by

$$\langle \vec{x} | n_x, n_y, n_z \rangle = \psi_{n_x,n_y,n_z}(\vec{x}) = \frac{1}{L^{3/2}} e^{2\pi i (n_x x + n_y y + n_z z)/L}. \tag{25}$$

n_x, n_y, and n_z are all integers to satisfy the required periodicity. The sum over states is given simply by the sum over these integer labels,

$$\sum_{n_x,n_y,n_z} \tag{26}$$

The momentum of the particle is given by the eigenvalues of the operators $\frac{\hbar}{i}\vec{\nabla}$, and therefore

$$\vec{p} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z). \tag{27}$$

Because we are interested in the large L limit, we can rewrite this sum as

$$\sum_{n_x,n_y,n_z} = \left(\frac{L}{2\pi\hbar}\right)^3 \sum_{n_x,n_y,n_z} \left(\frac{2\pi\hbar}{L}\right)^3. \tag{28}$$

We can identify $dp_x = \frac{2\pi\hbar}{L}$, $dp_y = \frac{2\pi\hbar}{L}$, and $dp_z = \frac{2\pi\hbar}{L}$. Taking the large L limit, the momentum becomes continuous, and the sum reduces to an integral,

$$\lim_{L\to\infty} \sum_{n_x,n_y,n_z} = \left(\frac{L}{2\pi\hbar}\right)^3 \int d\vec{p} = \int \frac{d\vec{x}d\vec{p}}{(2\pi\hbar)^3}. \tag{29}$$

In general, the sum over quantum states of a single particle is given by the *phase space* integral $d\vec{x}d\vec{p}$ with one state for each phase space volume $(2\pi\hbar)^D$ where D is the number of spatial dimension. In the presence of multiple particles, it would be

$$\prod_i \frac{d\vec{x}_i d\vec{p}_i}{(2\pi\hbar)^D}, \tag{30}$$

namely $(2\pi\hbar)^D$ for each particle. This is a result valid in any semi-classical limit where the levels can be considered approximately continuous.

Coming back to the scattering problem, we sum over the final states to define the probability of the outgoing particle to go into various momentum states,

$$\sum_f \Gamma(i \to f) = \int \frac{L^3 d\vec{p}_f}{(2\pi\hbar)^3} \frac{2\pi}{\hbar} \delta(E_i - E_f) |V_{fi}|^2 \tag{31}$$

Note that

$$V_{fi} = \langle f|V|i\rangle = \int d\vec{x} \frac{e^{-i\vec{p}_f \cdot \vec{x}/\hbar}}{L^{3/2}} V(\vec{x}) \frac{e^{i\vec{p}_i \cdot \vec{x}/\hbar}}{L^{3/2}} = \frac{1}{L^3} \int d\vec{x} V(\vec{x}) e^{i\vec{q}\cdot\vec{x}}, \tag{32}$$

where $\vec{q} = (\vec{p}_i - \vec{p}_f)/\hbar$. Therefore,

$$\sum_f \Gamma(i \to f) = \int \frac{d\vec{p}_f}{L^3 (2\pi\hbar)^3} \frac{2\pi}{\hbar} \delta(E_i - E_f) \left| \int d\vec{x} V(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2 \tag{33}$$

The cross section is defined by the number of scattered particles over the number incoming particles per unit area. The probability of finding a scattered particle is given by the rate times the time T, while the number of incoming particles per unit area is given by vT/L^3. In other words, the *flux* of the incoming particle is v/L^3 per unit time per unit area. Therefore the cross section is

$$\sigma = \frac{1}{v/L^3} \sum_f \Gamma(i \to f) = \frac{m}{p_i} \int \frac{d\vec{p}}{(2\pi\hbar)^3} \frac{2\pi}{\hbar} \delta(E_i - E_f) \left| \int d\vec{x} V(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2 \tag{34}$$

Next, we use $E_f = \frac{\vec{p}_f^2}{2m}$ and use the delta function $\delta(E_i - E_f) = \frac{m}{p_f} \delta(p_f - p_i)$,

$$\sigma = \frac{m^2}{p^2} \int \frac{p^2 d\Omega}{(2\pi\hbar)^3} \frac{2\pi}{\hbar} \left| \int d\vec{x} V(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2 = \int d\Omega \left| \frac{m}{\hbar^2} \frac{1}{2\pi} \int d\vec{x} V(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2. \tag{35}$$

This is nothing but the Born approximation for the cross section.

In general, the time-dependent perturbation theory at any given order gives the corresponding Born term at the same order in V, and the time-dependent perturbation theory and the time-independent formulation based on the Lippmann–Schwinger equation give the identical results.

4 Inelastic Scattering

4.1 Bethe–Bloch Formula for Energy Loss

What I did is covered by Sakurai. Consult Section 7.12.