Quantum Mechanics *H.T. 2001*

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Problem Set No. 8

Variational Principle

1. The functions $\phi_0, \phi_1, \phi_2, ...$ are a complete set of orthogonal and normalised eigenfunctions of a Hamiltonian $\hat{H}$ with energy eigenvalues $E_0 \leq E_1 \leq E_2 \leq .....$ respectively. Let ψ be an arbitrary normalised wavefunction, and let $\psi = \sum_n a_n \phi_n$.

   (i) Show that $\sum_n \mid a_n \mid^2 = 1$, and that

   $$\langle \psi \mid \hat{H} \mid \psi \rangle = \sum_n E_n \mid a_n \mid^2 .$$

   Show also that $\langle \psi \mid \hat{H} \mid \psi \rangle \geq E_0$.

   (ii) Explain what is meant by the *Variational Principle*, and show how it can be applied to give an upper bound to the true ground state energy of a quantum mechanical system.

   (iii) A particle of mass m moves in one dimension in the potential

   $$V(x) = \infty \quad (x \leq 0), \quad V(x) = ux \quad (x > 0)$$

   where u is a constant. Make a rough sketch of the wavefunctions for this particle in the ground and first excited states.

   (iv) Show that for a trial function of the form

   $$\psi(x) = 0 \quad (x \leq 0), \quad \psi(x) = Ax\exp(-ax) \quad (x > 0)$$

   the expectation value of the potential energy is $\langle \psi \mid V \mid \psi \rangle = 3u/2a$ and that of the kinetic energy operator is $\langle \psi \mid \hat{T} \mid \psi \rangle = \hbar^2 a^2/2m$. Hence obtain an estimate of the ground state energy.
   Explain why the true ground state wavefunction can be expected to fall off more rapidly than the trial wavefunction at large x.

Time-independent perturbation theory

2. Throughout this question the unperturbed Hamiltonian $\hat{H}_0$ is

   $$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

(a) Calculate the first order shift of the ground state energy caused by the perturbation $V_1 = \frac{1}{2}\beta x^2$, so that the Hamiltonian is $\hat{H}_0 + V_1$. Of course the ground state energy for $\hat{H}_0 + V_1$ can be found exactly using the standard results for the SHO; do this, expand it in powers of β, and compare with your perturbation theory result. You may quote any results you need about the eigenfunctions of $\hat{H}_0$ and any integral that may arise.

(b) Now consider $V_2 = -\alpha x$, so that the Hamiltonian is $\hat{H}_0 + V_2$. Show that the first order energy shift for *every* state is zero. Now solve the problem exactly. (Hint: to do this it is helpful (i) to sketch the full potential as a function of x and (ii) to re-express the Schrödinger equation in terms of $x' = x - b$ where b is a suitably chosen constant.) Is your result consistent with the first order perturbation theory calculation? What physical situation does this perturbation describe?

(c) Now consider the perturbation $V_3 = \lambda x^3$, so that the Hamiltonian is $\hat{H}_0 + V_3$. What is the first order energy shift for the ground state? Under what circumstances is this a true reflection of what happens to the ground state? (Hint: sketch the full potential.)

(d) **Outside the syllabus** The *second order* perturbation theory result for the energy shift is

$$\Delta E_n^{(2)} = \sum_{k \neq n} \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}.$$

Calculate this for V_2 (see part (b)). You will need

$$\int_{-\infty}^{\infty} dx\, \phi_k^*(x) x \phi_n(x) = \sqrt{\frac{\hbar}{2m\omega}} \begin{cases} \sqrt{n}, & \text{if } k = n-1; \\ \sqrt{n+1}, & \text{if } k = n+1; \\ 0, & \text{otherwise.} \end{cases}$$

Compare your result with the exact result from part (b). What does this tell you about the third, fourth, ... orders of perturbation theory for V_2?

3. In a more accurate treatment of the electron in the hydrogen atom, relativistic effects have to be taken into account. Here we'll calculate one of them. Starting from the relativistic energy–momentum relation for a free particle show that

$$E = mc^2 + \frac{p^2}{2m} - \frac{1}{2mc^2}\left(\frac{p^2}{2m}\right)^2 + \dots$$

Thus there is a relativistic correction to the kinetic energy operator

$$\Delta \hat{H} = -\frac{1}{2mc^2}\left(\frac{\hat{p}^2}{2m}\right)^2$$

Write down the formula which first order perturbation theory gives for the resulting shift in the energy E_n of the state $\phi_{n\ell m}$. It is tedious to compute the fourth derivative so use the time independent Schrodinger equation to eliminate the derivatives and obtain

$$\Delta E_n = -\frac{E_n^2}{2mc^2} \int dV \phi^*_{n\ell m} (1 - V(r)/E_n)^2 \phi_{n\ell m}$$

Show that the resulting first order shift in the ground state energy is $\Delta E_1 = -\frac{5}{2}(E_1/mc^2)E_1$. This answer has been written in the characteristic form "dimensionless number of order 1, which depends on the details of the calculation" $\times$ "dimensionless small quantity related to the perturbation" $\times$ "unperturbed energy scale". Why is E_1/mc^2 related to this particular perturbation? Evaluate ΔE_1 in eV.

[Harder: Compute ΔE_n for general n (you'll need to use a book to help with the integral). Is its dependence on n roughly what you'd expect?]

4. Using first order perturbation theory, calculate the shift in the ground state energy of a hydrogen-like atom due to the finite spatial extension of the nucleus, by the following method:
(a) Assuming that the nucleus is a sphere of radius R, and that its charge Ze is uniformly distributed throughout its volume, show that the potential energy of the electron is given by

$$\begin{aligned} V(r) &= -\frac{Ze^2}{4\pi\epsilon_0 R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right), \quad 0 \le r \le R \\ &= -\frac{Ze^2}{4\pi\epsilon_0 r}, \quad r \ge R \end{aligned}$$

where r is the distance of the electron from the centre of the nucleus.
(b) Apply first order perturbation theory by taking as perturbation the *difference* between $V(r)$ and the ordinary Coulomb potential i.e. write

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2\mu}\nabla^2 + V(r) \\ &= -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} + \left(V(r) + \frac{Ze^2}{4\pi\epsilon_0 r}\right) \\ &= \hat{H}_0 \text{ (hydrogenic) } + \text{ perturbation} \end{aligned}$$

where μ is the reduced mass of the electron. Sketch $V(r)$ and use your sketch to indicate how the *perturbation* varies with r. Note that the perturbation is zero for $r \ge R$, and that the unperturbed energies and wavefunctions are those of the hydrogenic problem.

Show that the shift in the ground state energy due to this perturbation is given approximately by

$$\Delta E = \frac{2}{5}\left(\frac{R^2}{a_Z^2}\right)\frac{Ze^2}{4\pi\epsilon_0 a_Z}$$

where $a_Z = \frac{4\pi\epsilon_0\hbar^2}{Z\mu e^2}$ (you may approximate e^{-r/a_Z} by 1 in the integral - why?).

Interpret the factors in ΔE along the lines of the discussion in Q.2. Evaluate ΔE in eV, taking $R = 1.0$ fm and $Z = 1$.

Suppose that, instead of an electron, a *muon* (mass = 105.658 MeV/c^2) were bound to the nucleus; what would ΔE be? (take the same values of R and Z).

5. *Refer back to the two-state problem of Set 7 question 1.*

(i)Show that for general E_1 and E_2 with $E_2 > E_1$, the exact eigenvalues are $E_\pm = (E_1 + E_2)/2 + \epsilon \pm [(E_2 - E_1)^2/4 + \epsilon^2]^{1/2}$. Also, find the ratio of (a/b) for each of these two energy eigenvalues.

(ii) Compare the expansion in powers of ϵ of your result, for both the energy eigenvalues and the ratios a/b, with the first order (in ϵ) perturbation formulae.

(iii) **Outside the syllabus** Now consider the case in which $E_1 = E_2 = 1$ so that the original (unperturbed) levels are *degenerate*. Again find the exact eigenvalues, and show that the exact eigenfunctions are $\phi_+ = \frac{1}{\sqrt{2}}(\phi_1 + \phi_2), \phi_- = \frac{1}{\sqrt{2}}(\phi_1 - \phi_2)$ (the $\frac{1}{\sqrt{2}}$'s are put in for normalization). Verify that

$$\int \phi_+^* V \phi_- = \int \phi_-^* V \phi_+ = 0$$

so that *using the functions ϕ_+ and ϕ_- as our "basis" functions*, V has "no-off diagonal matrix elements". Verify also that the exact energy eigenvalues are obtained by using the "first order perturbation theory" formula, but based on the wavefunctions ϕ_+ and ϕ_-.

This example introduces the general strategy to be adopted in handling perturbations applied to degenerate states (which is very frequently needed as the Atomic Physics course will show, for example). It is clear some special action *has* to be taken, if we look at the formula for the energy shift in ordinary second-order perturbation theory;

$$\Delta E_n^{(2)} = \sum_{m \neq n} \frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$$

where $V_{kn} = \int \phi_m^* V \phi_n$. The sum over "$n$" is over all states different from "m" - but what if one or more of those states had the same energy as "m"? This is exactly what degeneracy is - different wavefunctions having the same energy. In that case we will get a zero in the denominator, and the result is nonsense.

The reason for the nonsense is simple - perturbation theory is based on the approximation that the matrix elements of the perturbation are small compared with the energy differences between the unperturbed states; but if the latter can be *zero* the approximation can't get started! (But *perhaps* we would be OK if we used base states for which $V_{mn} = 0$ ...)

Note, however, that special action has to be taken *only* for the degenerate states; in general our unperturbed energy spectrum will contain many states which are not degenerate, and also some degeneracies. What we have to do is attack the degeneracies first, and then apply ordinary non-degenerate perturbation theory to the non-degenerate remaining states. The way to tackle the degenerate states is shown by the 2-state example above. For a certain energy level which is, say, r-fold degenerate in the absence of the perturbation V, with eigenfunctions $\phi_1, \phi_2, \ldots \phi_r$, we can solve the exact problem $(\hat{H}_0 + V)\phi = E\phi$ by writing $\phi = \sum_{n=1}^{r} a_n \phi_n$. This produces an $r \times r$ matrix problem, and r "exact" (within this space of degenerate levels) levels, and new wavefunctions which diagonalize V in this subspace. Quite often these new levels are no longer degenerate (as in the above example), though sometimes degeneracies can remain. See the T.T. course on Q.M. for Theory Option.

The Hamiltonian for a (spinless) electron of mass m interacting with a fixed charge of $+e$ at the origin, and with a constant magnetic field B in the z-direction is (see Set 5 Q 5)

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e}{2m}B\hat{L}_z$$

where $\hat{L}_z$ is the angular momentum operator. Treating the last term as a perturbation on the Coulomb hydrogenic problem, with hydrogen wavefunctions $R_{n\ell}(r)Y_{\ell m}(\theta, \phi)$, explain how a level of definite ℓ becomes split by the B-term. Calculate the splitting between the levels for $B = 1T$.

Explain why "ordinary" perturbation theory can be used, despite the fact that the unperturbed levels are degenerate. Can you find the *exact* eigenstates for H?

<u>A time-dependent problem: warm-up for time-dependent perturbation theory</u>

6. Consider a two-state system as in Q.4 above and Set 7 Q.1 , but now with the time-dependence included. There are two stationary states with wavefunctions $\psi_n = e^{-iE_n t/\hbar}\phi_n$, $(n = 1, 2)$ satisfying

$$i\hbar\frac{\partial \psi_n}{\partial t} = \hat{H}_0 \psi_n$$

with

$$\hat{H}_0 \phi_n = E_n \phi_n.$$

Now we add in a "potential" V, and try to solve

$$i\hbar\frac{\partial\psi}{\partial t} = (\hat{H}_0 + V)\psi.$$

As before, ψ can be expressed as a linear combination of the two (time-dependent) stationary state solutions, but this time the coefficients a and b will depend on t:

$$\psi = a(t)\phi_1 + b(t)\phi_2$$

(i) By following similar steps to those of Set 7 Q.1, show that

$$i\hbar\frac{da}{dt} = E_1 a + V_{11}a + V_{12}b$$

and

$$i\hbar\frac{db}{dt} = E_2 b + V_{21}a + V_{22}b$$

where

$$V_{ij} = \int \phi_i^* V \phi_j.$$

Note that if all the matrix elements of V were zero, equations (a) and (b) would "decouple" and the solutions would be just $a(t) = a(0)e^{-iE_1 t/\hbar}$, $b(t) = b(0)e^{-iE_2 t/\hbar}$, the expected stationary state behaviour for the Hamiltonian $\hat{H}_0$. The effect of the V_{ij}'s is to *couple* the amplitudes for the original stationary states. The problem is very similar to the normal mode problem in classical mechanics - in both cases, the "modes" are some linear combinations of the "coordinates" (here "a" and "b").

Note also that (a) and (b) have the general form

$$i\hbar\frac{d}{dt}\begin{pmatrix} a \\ b \end{pmatrix} = \boldsymbol{H}\begin{pmatrix} a \\ b \end{pmatrix}$$

where the matrix $\boldsymbol{H}$ is formed of the matrix elements of $\hat{H} = \hat{H}_0 + V$ in the ϕ_1, ϕ_2 basis via $\langle \phi_1 \mid \hat{H} \mid \phi_1 \rangle = E_1 + V_1$ etc. See Feynman Vol III chapters 8-11 for many variations on the "two-state" theme.

(ii) Consider a simple special case in which $E_1 + V_{11} = E_0 = E_2 + V_{22}$, and $V_{12} = V_{21} = V$ (real). The equations become

$$\begin{aligned} i\hbar\dot{a} &= E_0 a + Vb \\ i\hbar\dot{b} &= Va + E_0 b. \end{aligned}$$

Show that a solution can be found in which $a(t) = e^{-iEt/\hbar}\alpha$ and $b(t) = e^{-iEt/\hbar}\beta$, where α and β are constants, provided $E = E_0 \pm V$, and find α and β (normalized so that $\alpha^2 + \beta^2 = 1$) for each of the "modes" $E_+ = E_0 + V, E_- = E_0 - V$. Hence show that the two stationary states ("modes") for ψ are

$$\begin{aligned}\psi_+(t) &= e^{-iE_+t/\hbar}\left(\frac{1}{\sqrt{2}}\phi_1 + \frac{1}{\sqrt{2}}\phi_2\right)\\ \psi_-(t) &= e^{-iE_-t/\hbar}\left(\frac{1}{\sqrt{2}}\phi_1 - \frac{1}{\sqrt{2}}\phi_2\right).\end{aligned}$$

The energies $E_\pm$ are (of course?) the eigenvalues of the matrix $\boldsymbol{H}$ (compare the classical normal mode problem). The general solution to $i\hbar\frac{\partial\psi}{\partial t} = H\psi$ can be written as a linear superposition of our two "mode" solutions:

$$\psi(t) = A\psi_+(t) + B\psi_-(t)$$

with $\mid A \mid^2 + \mid B \mid^2 = 1$ and time-independent A and B. Verify this statement. Note that this *general* ψ is not a stationary wavefunction, in the sense that it does not have a definite energy and $\mid \psi(t) \mid^2$ does depend on t. The probability sloshes back and forth between "mode ψ_+" with energy E_+ and "mode ψ_-" with energy E_- (again, compare the general solution to a coupled oscillation problem).

Suppose the system is in the state such that $a(0) = 1, b(0) = 0$ (i.e. it is in state "ϕ_1" at $t = 0$). Show that the probability that it will be found to be in state ϕ_1 at a later time t is $\cos^2(Vt/\hbar)$. What is the probability that it will be found in state ϕ_2 at t?

Calculate the oscillation frequency $\omega = V/\hbar$ in s^{-1} for $V = 10^{-4}$ eV.

Time dependent perturbation theory

7. Let's return to the model of Q.6 (i) and set $V_{11} = V_{22} = 0$, so that $a(t)$ and $b(t)$ satisfy

$$\begin{aligned} i\hbar\dot{a} &= E_1 a + V_{12} b \\ i\hbar\dot{b} &= E_2 b + V_{21} a \end{aligned} \qquad (1)$$

Suppose now that the potential V is constant in time *except* that it is switched on suddenly at $t = 0$. So $V_{21} = V_{12} = 0$ for $t < 0$, $V_{12} = V_{12} = V$, say, for $t \geq 0$. Further, suppose that at $t = 0$, $a(0) = 1$ and $b(0) = 0$ so "it is in state ϕ_1". We want to solve (1) for "small" times and "small" V. First of all, we can get rid of the "diagonal" terms in E_1 and E_2 by simply writing

$$a(t) = c_1(t)e^{-iE_1t/\hbar}, b(t) = c_2(t)e^{-iE_2t/\hbar}.$$

Show that

$$\begin{aligned} (i) \quad i\hbar\dot{c}_1 &= Vc_2e^{i\omega_{12}t} \\ (ii) \quad i\hbar\dot{c}_2 &= Vc_1e^{-i\omega_{12}t} \end{aligned}$$

where $\omega_{12} = (E_1 - E_2)/\hbar$, and where $c_1(0) = 1, c_2(0) = 0$.

Show that, to first order in V,

$$\begin{aligned} c_2 &\approx \frac{V}{E_1 - E_2}[e^{-i\omega_{12}t} - 1] \\ c_1 &\approx 1. \end{aligned}$$

Hence show that the probability that the system will be found in state ϕ_2 at $t > 0$ is, in this approximation,

$$\frac{V^2}{\hbar^2}\left\{\frac{\sin^2(\omega_{12}t/2)}{(\omega_{12}/2)^2}\right\}.$$

[Optional: Actually, (i) and (ii) are simple enough to solve exactly: differentiate (ii) with respect to t, and obtain a second order equation for c_2; solve it subject to the boundary conditions $c_2(0) = 0, \dot{c}_2(0) = V_{21}c_1(0)/i\hbar = V_{21}/i\hbar$. Expand to lowest order in V to get the perturbation result back].

<u>Density of states</u>

This is something that you will use extensively in most of your courses over the next year; it is well worth taking the trouble to understand it properly. You'll need it for Q.9.

8. Consider a particle of mass m, in 1-D, confined to the region $0 \leq x \leq a$ by the "infinite-walled potential"; the energy levels are $E_n = n^2\pi^2\hbar^2/2ma^2$. Plot E_n (in units of $E_1 = \pi^2\hbar^2/2ma^2$) versus n for n up to 15. Consider an energy interval $\Delta E = 50$ in these units. Count the number of energy levels Δn in each successive such interval 0 to 50, 51 to 100, 101 to 150, etc. Δn changes with energy: plot $\Delta n/\Delta E$ versus the average energy $\bar{E}$ of each interval. This is called the "density of states" - the number of states per energy interval.

   It is clear that for something as light as a "microscopic" particle, if the size "a" of the confining region is "macroscopic" the energy levels will be so close together as to be effectively continuous (see Set 4 Q.6). So it will be a very good approximation to treat n as a continuous variable in $E(n) = n^2\pi^2\hbar^2/2ma^2 = n^2E_1$. By differentiating, show that in this "continuum limit" the number of energy levels dn per energy interval dE is

   $$\frac{dn}{dE} = \frac{1}{2E_1}\left(\frac{E_1}{E}\right)^{\frac{1}{2}}, \qquad (2)$$

   which is the (continuum) density of states for this 1-D case.

   Provided that "a" is such that 50 E_1 is still practically infinitesimal, we can say that our previous (discrete) density of states $\Delta n/\Delta E$ as a function of $\bar{E}$ should be approximately the same as the continuum version dn/dE. Measuring all energies in units of E_1, this means that (2) gives us $\Delta n/50 \approx 1/2\sqrt{E}$. Compare this with your earlier plot of $\Delta n/\Delta E$.

The above generalizes to 3-D by using the result of Set 4, Q.6: $E(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$, where n_x, n_y and n_z are positive integers. Consider "n-space" which is the 3-D space such that n_x is measured along one axis, n_y along a second and n_z along the third. Each energy eigenstate corresponds to one set of numbers (n_x, n_y, n_z) i.e. to a *point* in this "space". We want to calculate the number of these states dN per energy interval dE, i.e. the density of states dN/dE. Notice that if we introduce polar coordinates in n-space via $n_x = n\sin\theta\cos\phi$, $n_y = n\sin\theta\sin\phi$, $n_z = n\cos\theta$, then $E_n = n^2\pi^2\hbar^2/2ma^2$, so that all the states of a given energy lie on the surface of a sphere in the positive octant (since all n_x, n_y, n_z are > 0). So the total number of states is $N = \frac{1}{8}\frac{4\pi}{3}n^3$. Again, we will regard n and N as a continuous variables. As we change n to $n + dn$, we change E to $E + dE$ where $dE = \frac{\pi^2\hbar^2}{ma^2}ndn$ and N to $N + dN$ where $dN = \frac{\pi}{2}n^2dn$. Show that

$$\frac{dN}{dE} = \frac{2\pi V}{h^3}(2m)^{3/2}E^{1/2}$$

where $V = a^3$. Writing $dN = \text{constant} \times E^{\frac{1}{2}}dE$, what is the value of the constant if $a = 1$m, the particle is an electron, and energy is measured in joules?

Show that in 2-D, $\frac{dN}{dE} = \frac{2\pi Am}{h^2}$ where $A = a^2$.

9. Q.7 regards the potential, which is switched on at $t = 0$, as responsible for causing a *transition* from state ϕ_1 to state ϕ_2. For small t, $\mid c_2 \mid^2$ of Q.7 is proportional to t^2 ("$\sin^2 x \sim x^2$"), so that the transition probability per unit time is proportional to t. This is because we are dealing with a two-state system. Another common case in one in which there are very many states, which are very closely spaced together. This happens when we consider *scattering processes*, for example, where the states are classified (for one particle) by the momentum $\hbar\mathbf{k}$, and energies $\hbar^2\mathbf{k}^2/2m$. In such a case, we cannot speak of a transition to *one* particular state (since they form a continuum) but must instead find the probability for a transition to a *group* of states lying in the energy interval E to $E + dE$. Integrating the appropriate "$\mid c_f \mid^2$" over such a group of states produces a transition probability per unit time which is *independent* of time. It is called Fermi's Golden Rule:

$$\text{transition probability/unit time} = \frac{2\pi}{\hbar} \mid V_{fi} \mid^2 \frac{dN}{dE}$$

where $\frac{dN}{dE}$ is the density of final states about the energy E (see Q8).

Consider the application of this result to the scattering of a spinless particle by a potential $V(\mathbf{r})$. The states of the $V = 0$ problem are plane waves

$$\begin{aligned}\phi_i(\mathbf{r}) &= \frac{1}{L^{3/2}}e^{i\mathbf{k}_i.\mathbf{r}}\\ \phi_f(\mathbf{r}) &= \frac{1}{L^{3/2}}e^{i\mathbf{k}_f.\mathbf{r}}\end{aligned}$$

normalized in volume L^3.

(i) Prove that $\frac{dN}{dE} = \frac{mL^3}{8\pi^3\hbar^2}k \sin\theta d\theta d\phi$ where $k = \mid \mathbf{k}_i \mid = \mid \mathbf{k}_f \mid$ (elastic scattering) and θ, ϕ are the polar angles of $\mathbf{k}_f$.

(ii) Prove that the flux of incident particles is $\hbar\mathbf{k}_i/mL^3$, with magnitude $\hbar k/mL^3$.

(iii) The Golden Rule gives us the transition probability per unit time that, if we have one particle incident in a volume L^3, it will be scattered into a solid angle element $d\Omega = \sin\theta d\theta d\phi$. Call this $S(\theta)d\Omega$. The *differential cross section* is then defined as

$$\frac{d\sigma}{d\Omega} = S(\theta)/\text{incident flux}.$$

Consider the case $V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0|\mathbf{r}|}e^{-|\mathbf{r}|/a}$ (a "screened Coulomb" or "Yukawa" potential). The matrix element $< f \mid V \mid i >$ is

$$\begin{aligned}< f \mid V \mid i > &= \frac{1}{L^3}\int e^{-i\mathbf{k}_f.\mathbf{r}}\left(-\frac{e^2}{4\pi\epsilon_0}\frac{1}{\mid \mathbf{r} \mid}e^{-|\mathbf{r}|/a}\right)e^{i\mathbf{k}_i.\mathbf{r}}d^3\mathbf{r},\\ &= -\frac{e^2}{4\pi\epsilon_0 L^3}\int e^{i\mathbf{q}.\mathbf{r}}\frac{e^{-r/a}}{r}d^3\mathbf{r}\end{aligned}$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ and $r = \mid \mathbf{r} \mid$. Do the integral as follows: change to polar coordinates with the z axis chosen along $\mathbf{q}$ (which is "external" to the integral). Do the integral over θ. Then do the integral over r. Show that

$$< f \mid V \mid i > = -\frac{e^2}{\epsilon_0 L^3}\frac{1}{\mathbf{q}^2 + \frac{1}{a^2}}.$$

Now let $a \to \infty$ (the *Coulomb scattering case*) and show that

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{16\pi\epsilon_0 E}\right)^2\frac{1}{\sin^4\theta/2}$$

where θ is the angle between $\mathbf{k}_i$ and $\mathbf{k}_f$, and $E = \hbar^2k^2/2m$. This is the *Rutherford Scattering formula.*

Calculate $\frac{d\sigma}{d\Omega}$ (what are the *dimensions*?) for $E = 10$ keV and $\theta = 10°$.