

## Physics 4 - Quantum Physics 2000 - Problems.

### 1 Perturbation and Matrix Elements

Write down the wavefunctions  $|n\rangle$  for the bound states of an infinitely deep square well:  $V(-a < x < a) = 0$ ;  $V(-a > x > a) = \infty$ .

A perturbation  $\delta V(-a < x < a) = vx$  is added to the infinite square well potential. Under what conditions for  $v$  would it be appropriate to use perturbation theory.

Calculate the perturbed energies of the states and the matrix element between the two states with lowest energy.

By sketching the combination  $c_1|1\rangle + c_2|2\rangle$  show how mixing of state can allow more probability of the particle being in the region of lower potential  $x < 0$ . Similarly, show that the combination  $c_1|1\rangle + c_3|3\rangle$  can not achieve this.

What are the values of the matrix elements  $\langle 267|vx|387\rangle$  and  $\langle m|vx|m+738\rangle$ , where  $|m\rangle$  is the  $m^{\text{th}}$  lowest energy state?

### 2 Completeness and Orthonormality in Vectors and Basis Sets

Consider a unit vector  $\mathbf{a} = (1, 1, 3)/\sqrt{11}$ . What are its components (dot products) in the following 'basis sets'  $\mathbf{u}_i$ :

a)  $(1,0,0)$ ;  $(0,1,0)$ ;  $(0,0,1)$ .

b)  $(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0)$ ;  $(\frac{1}{2}, -\frac{\sqrt{3}}{2}, 0)$ .

c)  $(\frac{\sqrt{3}}{2}, 0, \frac{1}{2})$ ;  $(\frac{1}{2}, 0, \frac{\sqrt{3}}{2})$ ;  $(0,1,0)$ .

d)  $(\frac{\sqrt{3}}{2}, 0, \frac{1}{2})$ ;  $(\frac{1}{2}, 0, -\frac{\sqrt{3}}{2})$ ;  $(0,1,0)$ .

e)  $(2,1,-1)$ ;  $(1,0,2)$ ;  $(2,-5,-1)$ .

f)  $(-\frac{\sqrt{3}}{2}, 0, \frac{1}{2})$ ;  $(\frac{1}{2}, 0, \frac{\sqrt{3}}{2})$ ;  $(0,1,0)$ ;  $(\sqrt{\frac{2}{3}}, \sqrt{\frac{1}{6}}, -\sqrt{\frac{1}{6}})$ .

g)  $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$ ;  $(0,0,1)$

h)  $(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0)$ ;  $(\frac{1}{2}, -\frac{\sqrt{3}}{2}, 0)$ ;  $(-\sqrt{\frac{1}{2}}, -\sqrt{\frac{1}{2}}, 0)$ .

For each basis set, say whether it is complete, orthogonal and/or normalised. In each case evaluate  $\sum_i |\mathbf{a} \cdot \mathbf{u}_i|^2$  and  $u_i \cdot u_j$ . What is the general definition of a complete, orthonormal basis set in terms of these quantities? Can a basis set be overcomplete *and* orthonormal? Overcomplete *and* undercomplete?

For a calculation of electronic states in a hydrogen molecule, one may use a Fourier  $|\phi_{\mathbf{k}}\rangle = \exp(i\mathbf{k} \cdot \mathbf{r})$  or two sets of atomic hydrogen  $|\phi_{i,n,l,m}\rangle = |u_{n,l,m}(\mathbf{R}_i - \mathbf{r})\rangle$  basis set. Here  $\mathbf{k}$  is one of a set of wavevectors while  $\mathbf{R}_i$  are the nuclear positions. Sketch a typical basis function from each set. Discuss the completeness and orthogonality of these basis sets, and state an advantage that each has over the other.

### 3 One electron atoms

Look up and write down the  $n=1$  and  $2$  wavefunctions for a one electron atom (Nuclear charge  $Z$ ). Evaluate the first-order energy shifts and the matrix elements for the following perturbations:

a)  $v\hat{l}_z$

b)  $vr^2$

c)  $vr$

d)  $v \exp(-2r/a_0)$

e)  $v \exp(-Zr/a_0)$

In each case comment on the range of  $v$  for which perturbation theory is applicable.

## 4 Commutation

Calculate the following commutators:  $[\hat{p}_x, \hat{x}]$ ;  $[\hat{p}_x, \hat{y}]$ ;  $[\hat{l}_x, \hat{x}]$ ;  $[\hat{l}_x, \hat{y}]$ ;  $[\hat{p}_x, \hat{l}_x]$ ;  $[\hat{p}_x, \hat{l}_y]$ ;

What is the relationship between commutators and the uncertainty principle?

## 5 Spin-Orbit Coupling

Spin-orbit coupling arises from the interaction between the intrinsic (spin) magnetic moment of the electron and the magnetic field due to the moving charge. For a single electron, the form of the interaction is  $\eta \hat{\mathbf{l}} \cdot \hat{\mathbf{s}}$ .

Show that if the total angular momentum operator  $\hat{\mathbf{j}} = \hat{\mathbf{l}} + \hat{\mathbf{s}}$ , then the eigenvalues of  $\hat{\mathbf{l}} \cdot \hat{\mathbf{s}}$  are

$$\frac{1}{2}[J(J+1) - L(L+1) - S(S+1)]$$

Calculate the first order perturbation for the 1s, 2s and 2p states in hydrogen due to spin-orbit interaction in terms of  $\eta$ . Explain why these are *first-order* perturbations. Explain in terms of symmetry why the degeneracy of the six 2p levels is only partially lifted.

## 6 Degenerate Perturbation

A system  $\hat{H}_0$  has two degenerate eigenstates, which can be expressed as  $|\alpha_1\rangle$  and  $|\alpha_2\rangle$ . Show that  $\alpha(\theta) = (\cos\theta|\alpha_1\rangle + \sin\theta|\alpha_2\rangle)$  is also an eigenstate. What is the other eigenstate which makes up an orthonormal set with  $\alpha(\theta)$ ?

In the original eigenbasis, a measurable perturbation is defined by the matrix  $\langle\alpha_1|\hat{V}|\alpha_1\rangle = \langle\alpha_2|\hat{V}|\alpha_2\rangle = V_0$ , and  $\langle\alpha_1|\hat{V}|\alpha_2\rangle = V_1$ . What is  $\langle\alpha_2|\hat{V}|\alpha_1\rangle$ ? What is the splitting between the energies? What value of  $\theta$  corresponds to the nondegenerate eigenstates of  $\hat{H}_0 + \hat{V}$ ?

A system is prepared in state  $|\alpha_1\rangle$ . The perturbation is applied and then removed. What is the probability that the final state is  $|\alpha_2\rangle$ ? Why is it inappropriate to use time dependent perturbation theory here?

## 7 Good quantum numbers in hydrogen

Which of the following sets correspond to a complete commuting set of operators for hydrogen, and would therefore produce good quantum numbers for labelling a complete set of states. Explain why the other sets are bad. Assume that the hamiltonian excludes the spin orbit coupling term  $\xi \mathbf{L} \cdot \mathbf{S}$

- a)  $\hat{H}, \hat{L}^2, \hat{L}_z, \hat{L}_x$ .
- b)  $\hat{H}, \hat{L}^2, \hat{L}_z, \hat{J}_z$ .
- c)  $\hat{H}, \hat{S}^2, \hat{S}_z, \hat{J}_z$ .
- d)  $\hat{H}, \hat{x}, \hat{S}_z, \hat{J}_z$ .
- e)  $\hat{H}, \hat{L}^2, \hat{L}_z, \hat{J}_z, \hat{P}$  (parity).
- f)  $\hat{H}, \hat{L}^2, \hat{J}_z$ .
- g)  $\hat{H}, \hat{L}_z, \hat{S}_z, \hat{J}_z$ .
- h)  $\hat{H}, \hat{L}_z, \hat{S}^2, \hat{J}_z$ .
- i)  $\hat{H}, \hat{L}_z, \hat{S}^2, \hat{J}_z, \hat{S}_z$ .

## 8 Periodic perturbation

The degenerate wavefunctions for free particles in a 1D region of width  $L$  can be written  $\phi_{\pm} = L^{-1/2}e^{\pm ikx}$  (assume  $Lk \gg 1$ ).

What is the energy of particles described by these wavefunctions? Are the wavefunctions eigenfunctions of the Hamiltonian?

What is the expectation value of the momentum of particles described by these wavefunctions? Are the wavefunctions eigenfunctions of the momentum operator?

A weak periodic potential  $\hat{V}(x) = V_0 \cos(N\pi x/L)$  (with  $N$  very large) is applied. Evaluate the four matrix elements  $\langle \phi_{\pm} | \hat{V}(x) | \phi_{\pm} \rangle$ .

What are the perturbed energies of the states with  $|k| = N\pi/2L$  ?

Calculate the appropriate eigenstates of this potential. Are they eigenfunctions of the kinetic energy operator  $H_0 = -\hbar^2 \nabla^2 / 2m$  ?

Are they eigenfunctions of the momentum operator?

In which other course is this type of analysis of interest?

Consider energy shifts to second order in perturbation theory, in particular evaluate the matrix elements for mixing states with  $|k| = N\pi/2 \pm \delta$ .

## 9 Stark Effect

Consider the  $n=3$  levels of a hydrogen atom in an electric field. How many distinct non-zero matrix elements will there be in the Stark effect;  $\langle u_{3lm} | z | u_{3l'm'} \rangle \neq 0$ ?

## 10 Neutral kaons

Two operators which appear in particle physics are charge conjugation ( $\hat{C}$ ), which reverses the sign of the charge and the magnetic moment of a particle, and parity ( $\hat{P}$ ) which inverts space  $\mathbf{r} \rightarrow -\mathbf{r}$ . A combination of these two is called CP. To calculate decay via the weak interaction, we need to consider  $\hat{C}\hat{P}$  eigenstates.

The neutral kaon states produced by pion decay via the strong interaction are  $|K^0\rangle$  and  $|\bar{K}^0\rangle$ , eigenvalues of strangeness  $\hat{S}$  such that  $\hat{S}|K^0\rangle = |K^0\rangle$  and  $\hat{S}|\bar{K}^0\rangle = -|\bar{K}^0\rangle$ . Acting on these states with  $\hat{C}\hat{P}$  gives:

$$\hat{C}\hat{P}|K^0\rangle = |\bar{K}^0\rangle; \quad \hat{C}\hat{P}|\bar{K}^0\rangle = |K^0\rangle$$

Evaluate the CP eigenstates for neutral kaons. These are called  $|K_1\rangle$  and  $|K_2\rangle$ . Show that they have eigenvalues CP=+1 and CP=-1 respectively.

The lifetime of  $|K_1\rangle$  is  $\tau_1 = 0.9 \times 10^{-10}$  and the lifetime of  $|K_2\rangle$  is  $\tau_2 = 0.5 \times 10^{-7}$ .

By evaluating the time dependence of the probability amplitude  $|a_1(t)|^2$ , show that the time dependent wavefunction  $a_1(t) = a_1(0)e^{-t/2\tau_1}e^{-ixt}$ , where  $x$  is any real number, represents decay with lifetime  $\tau$ .

Thus show that the time-dependent amplitudes of the  $|K_1\rangle$  and the  $|K_2\rangle$  states ( $a_1(t)$  and  $a_2(t)$  respectively) at rest (i.e. with  $E = mc^2$ ) are given by:

$$a_1(t) = a_1(0)e^{-t/2\tau_1}e^{-im_1c^2t/\hbar} \quad \text{and} \quad a_2(t) = a_2(0)e^{-t/2\tau_2}e^{-im_2c^2t/\hbar}$$

Show that the intensity of  $|K^0\rangle$  is measured by the operator  $\frac{1}{2}(\hat{S} + 1)$ . What is the operator for the intensity of  $|\bar{K}^0\rangle$ ?

If at  $t=0$  a kaon beam is in a pure  $|K^0\rangle$  state, with intensity proportional to  $|a_0(0)|^2 = 1$  show that at time  $t$

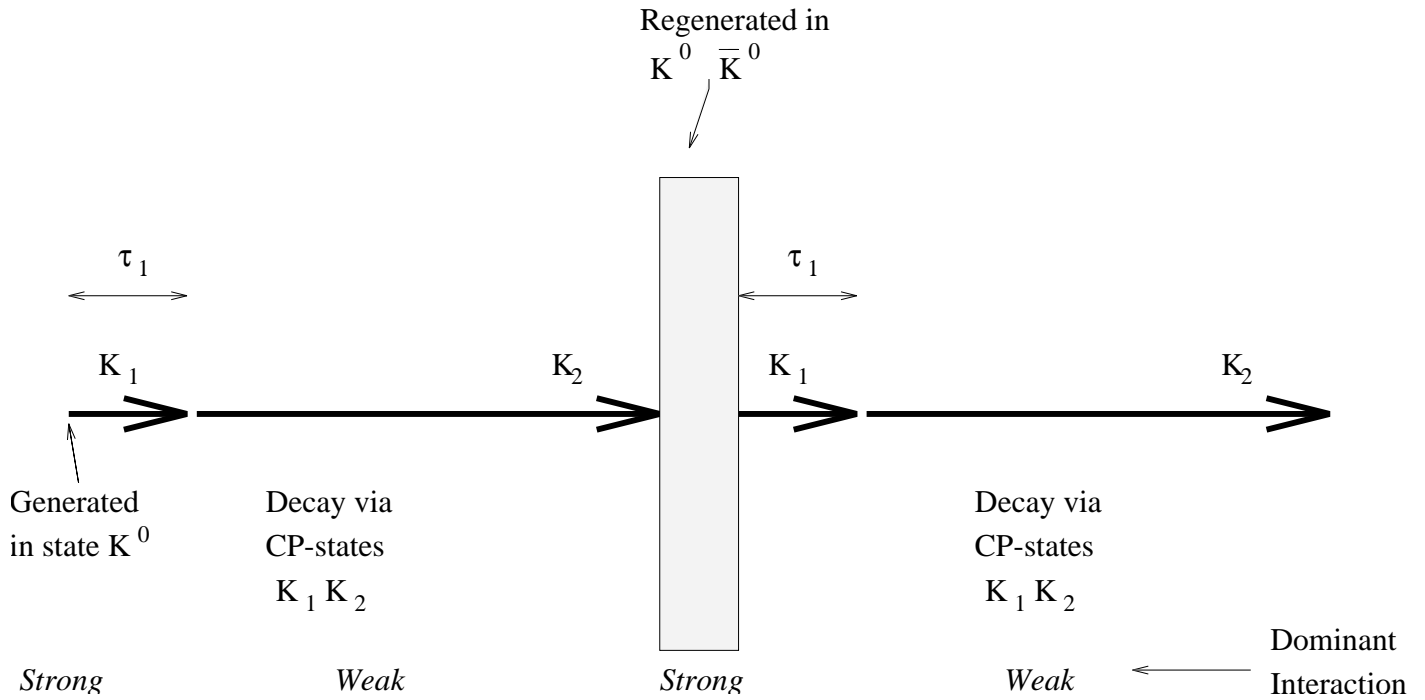


Figure 1: Appropriate basis states for neutral kaons

$$|a_0(t)|^2 = \langle \frac{1}{2}(\hat{S} + 1) \rangle = \frac{1}{4} [e^{-t/\tau_1} + e^{-t/\tau_2} + 2e^{-t/2\tau_1} e^{-t/2\tau_2} \cos(m_{12}t)]$$

and

$$I(\bar{K}^0) = \frac{1}{4} [e^{-t/\tau_1} + e^{-t/\tau_2} - 2e^{-t/2\tau_1} e^{-t/2\tau_2} \cos(m_{12}t)]$$

where  $m_{12} = (m_2 - m_1)c^2/\hbar$ . Note that intensities are unchanged if we use  $m_{12} = (m_1 - m_2)c^2/\hbar$  - is there a physical reason for this?

Sketch, as a function of time, the expectation values of:  $\frac{1}{2}(\hat{S} + 1)$ ,  $\hat{S}$ ,  $\hat{S}^2$ ,  $\hat{C}P$ ,  $\frac{1}{2}(\hat{C}P + 1)$  in a system which began in state  $|K^0\rangle$ .

Figure 1 shows a kaon beam experiment. The kaons are generated in state  $|K^0\rangle$ . After  $10^{-9}$  seconds the kaons pass through a small region of matter, where they interact via the strong interaction (you may assume that after  $10^{-9}$  seconds all the  $|K_1\rangle$  particles have decayed).

Very soon after, the kaons leave the matter and move into a region of vacuum where they begin to decay via the weak interaction. Assume that all coherence between this region and the previous region is lost i.e. the wavefunction is completely collapsed onto its strong interaction eigenstates. Evaluate the appropriate eigenstates and intensities just before the beam enters the matter and just after it leaves the matter. What is the total intensity of kaons and antikaons which survive a further  $10^{-9}$  seconds?

Had it not been for the matter, what would have been the total intensity of kaons and antikaons after  $2 \times 10^{-9}$ ? The effect of the matter on the beam is known as regeneration.

Compare figure 1 to a system of polarisers and light beams.

*Note* The regeneration here is known as incoherent regeneration, because the wavefunction is collapsed in the matter and all 'memory' of the previous state is lost. In practice there is also an effect known as coherent regeneration, in which a difference between the amount of scattering of  $|K^0\rangle$  and  $|\bar{K}^0\rangle$  leads to a component of  $|K_1\rangle$  being reintroduced.

## 11 Variational principle

Estimate the energy of the ground state of a 1D harmonic oscillator using as a trial function:

a)  $\cos ax$  (for  $|ax| < \pi/2$ , zero elsewhere)

b)  $a^2 - x^2$  (for  $|x| < a$ , zero elsewhere)

c)  $Ae^{-\alpha x^2}$

d)  $C(a - |x|)$  (for  $|x| < a$ , zero elsewhere)

e)  $\sin ax$  (for  $|ax| < \pi$ , zero elsewhere)

Don't forget the normalisation. Sketch the wavefunctions and compare them with the actual ground state wavefunction.

Write down the overlap integral between the wavefunction in (e) and each of the other four: Why does (e) represent an estimate of the first excited state?

Where does the kinetic energy come from in (d)?

You may use the results:  $\langle (a - |x|) | \frac{d^2}{dx^2} | (a - |x|) \rangle = -\pi a$

$$\int_{-\pi/a}^{\pi/a} x^2 \sin^2 ax \, dx = \pi(2\pi^2 - 3)/6a^3$$

$$\int_{-\pi/2a}^{\pi/2a} x^2 \cos^2 ax \, dx = \pi(\pi^2 - 6)/24a^3$$

## 12 Degenerate Perturbation

A two dimensional infinite square well has potential:  $V(|x| < L, |y| < L) = 0; V = \infty$  elsewhere

Write down the solutions to the Schroedinger equation for this potential.

What symmetries does this potential have? Consider applying the symmetry elements of the potential to the wavefunctions, how does the symmetry relate to degeneracy?

A perturbation  $\delta V = vxy$  is applied. How does this effect the symmetry? Consider the (degenerate) first excited state of the potential. What are the appropriate basis states which are eigenstates of this potential? What are the shifts in energy of the first excited states due to the perturbation?

You may wish to use the result:  $\int_{-\pi/2}^{\pi/2} \theta \sin 2\theta \cos \theta \, d\theta = 8/9$

## 13 Properties of Legendre Polynomials

The solution to the 3D Schroedinger Equation with a central potential involves Legendre polynomials. Make sure you know what they are. Look up and write down the first five Legendre polynomials  $P_l(\cos \theta)$ .

For each combination of  $l$  and  $m$  up to 3, evaluate

$$\int_0^\pi P_l(\cos \theta) P_m(\cos \theta) \sin \theta \, d\theta$$

The substitution  $x = \cos \theta$  may be useful. For  $l = 0, 1, 2$  and 3, evaluate  $P_l(1)$  and  $P_l(0)$ .

Verify that  $P_l(-x) = (-1)^l P_l(x)$ . In atoms, what operator has eigenvalues  $(-1)^l$ ?

Verify for  $l = 1, 2$  and 3 that

$$\cos \theta P_l(\cos \theta) = \frac{l+1}{2l+1} P_{l+1}(\cos \theta) + \frac{l}{2l+1} P_{l-1}(\cos \theta)$$

How does this result affect transitions between atomic energy levels in the dipole approximation, where the perturbation is written as  $eE_z \cos \theta$ ?

## 14 Abstract Operators

If the proton and neutron are represented by eigenvectors  $|p\rangle = [1\ 0]$  and  $|n\rangle = [0\ 1]$ , what 2x2 matrix operator  $\hat{Q}$  would represent charge (take the proton charge to be  $e=1$ )?

What are the eigenvectors and eigenvalues of a matrix operator  $\hat{T}_3 = 2\hat{Q} - \hat{I}$ , where  $\hat{I}$  is the identity matrix?

To describe a proton decaying to a neutron, we introduce an operator  $\hat{T}_1$  for which  $\hat{T}_1|p\rangle = |n\rangle$  and  $\hat{T}_1|n\rangle = |p\rangle$ . What is the matrix representation of  $\hat{T}_1$ ? What is the expectation value of the charge for the eigenstates of  $\hat{T}_1$ ?

In what other course do these  $\hat{T}$  operators occur, and what are they called?

## 15 Density of states - Born Approximation

By analogy with the 1d infinite square well, write down the allowed wavefunctions for a particle in a large cubic box. How many allowed states are there with energies between  $E$  and  $E + dE$ ? How many allowed states are there with both energy between  $E$  and  $E + dE$  and wavevector at an angle between  $\theta$  and  $\theta + d\theta$  to the z-axis? What does this have to do with the Born Approximation?

## 16 Impact parameters

Calculate the classical impact parameter for a 1eV  $p$ -electron and discuss the energy range in which the  $s$ -wave approximation is reasonable for atomic scattering.

## 17 Partial Waves

The phase shifts for free electrons scattered by a particular potential are given as a function of energy (in electron volts) approximately by:

$$\delta_0 = \pi + \pi \exp\left(\left[1 - 4(E - 0.5)^2\right]/8\right) \quad \delta_l = (E/10)^l \pi/2 \quad (l \leq 5); \quad \delta_n = 0, \quad (l \geq 6).$$

Sketch the function  $\delta_0(E)$ .

How many bound states does this potential have?

At what energy will there be a sharp minimum in the total scattering cross section (the Ramsauer effect)? At what energies above this could there be maxima due to  $s$ -wave scattering? At what energy could there be a maximum in the  $p$ -wave scattering? Which of these features could be observed experimentally?

At approximately what energy is the total scattering strongest  $\sigma_{max}$ , and what approximate value will it have relative to the  $s$ -wave peak?

How does the scattering cross-section vary with energy at high energy?

It is instructive to generate plots of  $\sigma(E)$  using maple.

## 18 Atomic Scattering

For the case of high energy scattering of an electron by an atom, with electron probability density  $\rho(r)$  we approximate the potential by

$$V(r) = \frac{-Ze^2}{4\pi\epsilon_0 r} + \int \int \int \frac{\rho(r_Z)e^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}_Z|} d^3\mathbf{r}_Z$$

Sketch the first term of this potential against  $r$ . What does it represent? On the same graph, sketch a reasonable form of the second term of this potential. What does it represent?

Finally, still on the same graph, sketch a reasonable form of the total potential against  $r$ . Include the appropriate length scale.

Write down the integral required to evaluate the scattering cross section in the Born approximation.

Given that the ‘Bethe integral’, is  $\int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r} d^3\mathbf{r} = 4\pi/k^2$ , show that the Born integral associated with this potential (i.e. Fourier transform) is:

$$\frac{e^2}{\epsilon_0\chi^2}[-Z + F(\chi)]$$

where  $F(\chi) = \int e^{i\chi\cdot\mathbf{r}}\rho(\mathbf{r})d^3\mathbf{r}$  is called the *form factor* for the atom; it is the Fourier transform of the charge density. [Hint: use the substitution  $\mathbf{x} = \mathbf{r} - \mathbf{r}_Z$ ]

In what other course does this form factor occur?

Write down the scattering cross section for this potential, both in terms of the electron wavevector  $k$  and in terms of its velocity  $v = \hbar k/m$ .

Referring back to your sketch graph for  $V(r)$ , estimate the electron energy below which  $s$ -wave scattering would be a good description.

## 19 Coulomb Scattering

Using results from the previous question, show that the scattering cross section from a bare nucleus is:

$$\frac{d\sigma}{d\Omega} = \left( \frac{Ze^2}{4\pi\epsilon_0 2\mu v^2 \sin^2 \frac{\theta}{2}} \right)^2.$$

What is unusual in its absence in this *quantum* expression. Where have you seen this before? Why might you expect the Born approximation to give the wrong answer for this problem? (Don’t worry, in fact the answer is correct).

## 20 Hydrogen Scattering

For hydrogen, the charge density is simply the square of the wavefunction:

$$\rho(r) = (1/\pi a_0^3) \exp(-2r/a_0)$$

Show that the form factor for this is  $F(k) = [1 + a_0^2 k^2 \sin^2 \frac{\theta}{2}]^{-2}$ . (Quite tricky integration)

and thus that in the Born Approximation:

$$\frac{d\sigma}{d\Omega} = \frac{a_0^2 (2 + a_0^2 k^2 \sin^2 \frac{\theta}{2})^2}{4 (1 + a_0^2 k^2 \sin^2 \frac{\theta}{2})^4}$$

Sketch this function.

## 21 Centre of mass coordinates

Write down the one dimensional Schroedinger equation for two distinguishable particles with positions  $x_1$  and  $x_2$  interacting with one another via a potential  $V(|x_1 - x_2|)$ .

Show that this equation can be separated into two ‘effective particle’ equations by the substitutions

$$r = x_1 - x_2; \quad R = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

## 22 Imaginary potentials

Solve the time dependent Schrodinger equation for a particle moving in a region of constant potential  $V(x, t) = V_0 + iV_1$ . Evaluate the probability current density. Discuss what this might mean physically. Likewise, discuss the particle in potential  $V(x, t) = V_0 - iV_1$ . Why is this at best only a partial description of a real system.

## 23 Electron-electron Scattering

Using the result obtained for Coulomb scattering, calculate and plot graphs of  $\frac{d\sigma}{d\Omega}$  vs  $\theta$  for the differential scattering cross section of two colliding beams of 1eV electrons with:

(a) Opposite spins. (b) Identical spins. (c) Unpolarised spins.

## 24 Bell's Theory

Two photons travel in opposite directions toward two linear polarisers A and B at angles  $\theta_A$  and  $\theta_B$  to the z-axis. What is the probability that both pass through if they are:

(a) Uncorrelated - produced by different sources.

(b) Produced in an uncorrelated state polarised in the z-direction.

(c) Produced in a correlated state with opposite polarisations from a spherically symmetric source.

Two electrons travel in opposite directions and are deflected by two Stern Gerlach apparatuses, A and B at angles  $\theta_A$  and  $\theta_B$  to the z-axis. What is the probability that "spin up" is measured by both apparatus (i.e. one spin  $\frac{1}{2}$  points along  $\theta_A$  and the other along  $\theta_B$ ) if the electrons are:

(d) Uncorrelated - produced by different sources.

(e) Produced in a correlated state with opposite polarisations from a spherically symmetric source.

Explain why (c) and (e) give different answers. Which cases would be different in the 'hidden variables' interpretation of quantum mechanics?

What, in each case, are the average probabilities taken over all angles  $\theta_A$  and  $\theta_B$ ?

## 25 Kronig-Penney

In the Kronig-Penney model, the energy of an electron with wavenumber  $k$  is given in section 4.5 of the notes. What happens when  $l = b$ ? What happens when  $b = 0$ ? What is the physical interpretation of these limits?

## 26 Hydrogen Molecular Ion

A system comprises two protons and an electron. When the protons are widely separated show that the ground state for the electron is doubly degenerate (ignore spin).

Using these two states as basis states when the protons are a distance  $R$  apart, show that the integrals involved in the matrix elements  $V_{11}$  and  $V_{12}$  required in a degenerate perturbation treatment are:

$$\int \frac{e^{2r/a_0}}{|\mathbf{r} - \mathbf{R}|} d^3\mathbf{r} \quad \text{and} \quad \int \frac{e^{r/a_0} e^{|\mathbf{r} - \mathbf{R}|/a_0}}{r} d^3\mathbf{r}$$

Sketch the matrix elements integrals as a function of  $R$ .

In terms of the matrix elements what are the energies of the perturbed states? Explain why the electron provides an attractive force between the protons. What is the approximation that makes this a perturbation theory, and when will it break down?



## Some Integrals

$$\int_{-a}^a (\text{Any odd function}) dx = 0$$

$$\int_0^a x \cos^2\left(\frac{n\pi x}{2a}\right) dx = \frac{a^2}{4} \left[1 - \frac{4}{n^2\pi^2}\right] \quad n \text{ odd} \quad ; \quad \int_0^a x \sin^2\left(\frac{n\pi x}{2a}\right) dx = \frac{a^2}{4} \left[1 + \frac{4}{n^2\pi^2}\right] \quad n \text{ odd}$$

$$\int_0^a x \sin^2\left(\frac{n\pi x}{2a}\right) dx = \int_0^a x \cos^2\left(\frac{n\pi x}{2a}\right) dx = \frac{a^2}{4} \quad n \text{ even}$$

$$\int_{-\pi/2}^{\pi/2} x \cos^2 x \sin x dx = \frac{4}{9}$$

$$\int_0^\infty x^n \exp(-ax) dx = n! a^{-(n+1)}$$

$$\int_0^L \cos^2(\pi x/L) dx \int_0^L \sin^2(\pi x/L) dx = L/2$$

$$\int_{-\pi/a}^{\pi/a} x^2 \sin^2 nax dx = \frac{\pi(2n^2\pi^2 - 3)}{6n^2a^3} \quad ; \quad \int_{-\pi/a}^{\pi/a} x^2 \cos^2 nax dx = \frac{\pi(2n^2\pi^2 + 3)}{6n^2a^3}$$

$$\int_{-a}^a a^4 - 2a^2x^2 + x^4 dx = \frac{16}{15}a^5$$

$$\int_{-\infty}^{\infty} x^2 \exp(-x^2/\sigma^2) dx = \frac{\sigma^3\sqrt{\pi}}{2}$$

$$\int_{-\infty}^{\infty} \exp(-x^2/\sigma^2) dx = \sigma\sqrt{\pi}$$

$$\int_0^a x^2(x-a)^2 dx = \frac{a^5}{30}$$

$$\int_{-\pi/2}^{\pi/2} \sum_{n=1}^{\infty} \frac{\cos^2 nx}{n^2} dx = \frac{\pi^3}{16}$$

$$\int_{-\infty}^{\infty} d^3\mathbf{x} \int_{-\infty}^{\infty} d^3\mathbf{y} \frac{\rho(x) \exp(-i\mathbf{k}\cdot\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} = \int_{-\infty}^{\infty} d^3\mathbf{x} \int_{-\infty}^{\infty} d^3\mathbf{z} \frac{\rho(x) \exp -i\mathbf{k}\cdot(\mathbf{x}+\mathbf{z})}{|\mathbf{z}|} = \frac{4\pi}{k^2} \int_{-\infty}^{\infty} d^3\mathbf{x} \rho(x) \exp -i\mathbf{k}\cdot\mathbf{x}$$

$$\int_0^\infty x \exp(-2x/a) \cos(\chi x) dx = \frac{a^2(\chi^2 a^2 - 4)}{(\chi^2 a^2 + 4)^2}$$