

Quantum Physics 2011/12

Solutions to Tutorial Sheet 3: More Perturbations

1. *Quarkonium is a system consisting of a heavy quark of mass m_Q bound to its antiquark, also of mass m_Q . The inter-quark potential is of the form*

$$V(r) = -\frac{a}{r} + br ,$$

where a, b are constants and r is the quark-antiquark separation. Given the Bohr formula for the energy levels of hydrogen

$$E_n^{(0)} = -\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{n^2} ,$$

where m is the reduced mass of the electron-proton system, deduce an expression for the energy levels of quarkonium in the approximation which neglects the second term in $V(r)$.

The Hamiltonian which describes the system in the centre-of-mass frame is

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 + V(r)$$

where $\mu = m_Q/2$ is the reduced mass of the quark-antiquark system.

Dropping the linear term in the potential means that the problem reduces to that of a hydrogen-like system with Hamiltonian

$$\hat{H}_0 = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{a}{r}$$

Thus we can use the Bohr formula to write down the energy eigenvalues if we make the replacements

$$\frac{e^2}{4\pi\epsilon_0} \rightarrow a \quad \text{and} \quad m \rightarrow \frac{m_Q}{2}$$

giving

$$E_n^{(0)} = -\frac{m_Q}{4\hbar^2} \frac{a^2}{n^2}$$

What are the corresponding degeneracies of the lowest two energy levels?

The corresponding eigenfunctions are labelled by the usual quantum numbers n, ℓ, m_ℓ if we ignore spin. For each value of ℓ , there are $(2\ell + 1)$ values of m_ℓ . Since the quark and antiquark each have $s = 1/2$, the total spin $S = 1$ or 0 , so that there are four possible spin states, (three triplet and one singlet). Thus the degeneracies of the lowest two energy levels with $n = 1$ and $n = 2$ are as follows.

When $n = 1$, $\ell = m_\ell = 0$, $S = 1$ or 0 so the degeneracy is fourfold.

When $n = 2$, $\ell = m_\ell = 0$ or $\ell = 1$, $m_\ell = 1, 0, -1$, $S = 1$ or 0 and so the degeneracy is sixteenfold.

Aside: the quantum numbers ℓ and m_ℓ relate to the *relative* orbital angular momentum of the two-particle, quark-antiquark system and are here denoted by capital letters: L and M_L , rather than the lower-case, one-electron notation. Of course, strictly even the electron-proton system has ℓ quantised for the whole system, but the difference in masses makes it reasonable to associate ℓ with the electrons, and this becomes useful when there are more than one electron.

Use first-order perturbation theory to calculate the corrections to the lowest two energy levels. Why it is not necessary to use degenerate perturbation theory for this problem?

You may assume that the radial functions for hydrogen are:

$$\begin{aligned} R_{10} &= 2(a_0)^{-3/2} \exp(-r/a_0) \\ R_{20} &= 2(2a_0)^{-3/2} \left(1 - \frac{r}{2a_0}\right) \exp(-r/2a_0) \\ R_{21} &= \frac{1}{\sqrt{3}}(2a_0)^{-3/2} \frac{r}{a_0} \exp(-r/2a_0) \end{aligned}$$

where the Bohr radius $a_0 = 4\pi\epsilon_0\hbar^2/me^2$, and that

$$\int_0^\infty \exp(-kr) r^n dr = n!/k^{n+1}, \quad n > -1$$

We treat the linear term in \hat{H} as a perturbation by writing

$$\hat{H} = \hat{H}_0 + \Delta\hat{V}$$

In first-order perturbation theory, the correction to the k^{th} state is

$$\Delta E_k = \langle k | \Delta\hat{V} | k \rangle$$

where the label k is shorthand for the complete set of quantum numbers n, L, M_L, S, M_S needed to specify fully the eigenstates of the unperturbed Hamiltonian \hat{H}_0 . The eigenfunctions are of the form

$$u_{nLM_L}(\underline{r}) = R_{nL}(r)Y_{LM_L}(\theta, \phi)$$

where the radial functions $R_{nL}(r)$ are obtained from the corresponding hydrogenic functions by making the replacement

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \rightarrow \frac{2\hbar^2}{am_Q}$$

For the present problem, the perturbation contains no spin operators and so we can ignore the labels S and M_S . Furthermore, it is independent of direction and so there is no dependence on the magnetic quantum number M_L :

$$\Delta E_{nL} = b \int_0^\infty r R_{nL}^2(r) r^2 dr \int \int |Y_{LM_L}(\theta, \phi)|^2 \sin\theta d\theta d\phi$$

Since the spherical harmonics are normalised, the second integral is unity and thus the first-order correction reduces to

$$\Delta E_{nL} = b \int_0^\infty r R_{nL}^2(r) r^2 dr$$

Using the given radial functions:

$$\begin{aligned}
\int_0^\infty r R_{10}^2(r) r^2 dr &= \frac{4}{a_0^3} \int_0^\infty r^3 \exp(-2r/a_0) dr = \frac{3a_0}{2} \rightarrow \frac{3\hbar^2}{am_Q} \\
\int_0^\infty r R_{20}^2(r) r^2 dr &= \frac{1}{4a_0^3} \int_0^\infty r^3 \left(1 - \frac{r}{2a_0}\right)^2 \exp(-r/a_0) dr \\
&= \frac{1}{4a_0^3} \left\{ \int_0^\infty r^3 \exp(-r/a_0) dr - \int_0^\infty \frac{r^4}{a_0} \exp(-r/a_0) dr \right. \\
&\quad \left. + \int_0^\infty \frac{r^5}{4a_0^2} \exp(-r/a_0) dr \right\} = 6a_0 \rightarrow \frac{12\hbar^2}{am_Q} \\
\int_0^\infty r R_{21}^2(r) r^2 dr &= \frac{1}{24a_0^3} \int_0^\infty \frac{r^5}{a_0^2} \exp(-r/a_0) dr = 5a_0 \rightarrow \frac{10\hbar^2}{am_Q}
\end{aligned}$$

Thus the desired first-order corrections are

$$\Delta E_{10} = \frac{3b\hbar^2}{am_Q}, \quad \Delta E_{20} = \frac{12b\hbar^2}{am_Q}, \quad \Delta E_{21} = \frac{10b\hbar^2}{am_Q}$$

The perturbation $\Delta\hat{V} = br$ is spherically symmetric which means that

$$[\Delta\hat{V}, \hat{L}^2] = [\Delta\hat{V}, \hat{L}_z] = 0$$

so that the quantum numbers L and M_L remain good quantum numbers in the presence of the perturbation. In other words, off-diagonal matrix elements of $\Delta\hat{V}$ in the basis $\{n, L, M_L\}$ must vanish for a given n as is readily established:

$$\langle n, L', M'_L | [\Delta\hat{V}, \hat{L}^2] | n, L, M_L \rangle = \{L'(L'+1) - L(L+1)\} \hbar^2 \langle n, L', M'_L | \Delta\hat{V} | n, L, M_L \rangle = 0$$

which implies that for $L' \neq L$

$$\langle n, L', M'_L | \Delta\hat{V} | n, L, M_L \rangle = 0$$

Similarly,

$$\langle n, L', M'_L | [\Delta\hat{V}, \hat{L}_z] | n, L, M_L \rangle = \{M'_L - M_L\} \hbar \langle n, L', M'_L | \Delta\hat{V} | n, L, M_L \rangle = 0$$

Alternatively, a statement that the corresponding spherical harmonics are orthogonal would be acceptable.

Since the off-diagonal matrix elements of $\Delta\hat{V}$ vanish, the perturbation is diagonal in the chosen basis, implying that the first-order energy shifts are just given by the formula of non-degenerate perturbation theory.

2. *The isotropic harmonic oscillator in 2 dimensions is described by the Hamiltonian*

$$\hat{H}_0 = \sum_i \left\{ \frac{\hat{p}_i^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}_i^2 \right\} \quad i = 1, 2$$

and has energy eigenvalues

$$E_n = (n+1)\hbar\omega \equiv (n_1 + n_2 + 1)\hbar\omega \quad n = 0, 1, 2, \dots$$

What is the degeneracy of the first excited level? Use degenerate perturbation theory to determine the splitting induced by the perturbation

$$\Delta\hat{V} = Cx_1x_2$$

where C is a constant.

Hint: the matrix elements of the perturbation may be computed by using the lowering and raising operators

$$\hat{a}_i \equiv \sqrt{\frac{m\omega}{2\hbar}} \hat{x}_i + \frac{i}{\sqrt{2m\omega\hbar}} \hat{p}_i \quad \text{and} \quad \hat{a}_i^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}} \hat{x}_i - \frac{i}{\sqrt{2m\omega\hbar}} \hat{p}_i$$

with the properties that

$$\hat{a}_1|n_1, n_2\rangle = \sqrt{n_1}|n_1 - 1, n_2\rangle \quad \text{and} \quad \hat{a}_1^\dagger|n_1, n_2\rangle = \sqrt{n_1 + 1}|n_1 + 1, n_2\rangle \quad \text{etc.}$$

The first excited level corresponds to $n = 1$ which can clearly be obtained in two possible ways: $n_1 = 1, n_2 = 0$ or $n_1 = 0, n_2 = 1$. Thus the first excited level is 2-fold degenerate. In an abbreviated notation we can label the corresponding states $|10\rangle$ and $|01\rangle$.

To calculate the splitting induced by the perturbation we must evaluate the matrix elements of $\Delta\hat{V}$ between these states:

$$C \begin{pmatrix} \langle 10|x_1x_2|10\rangle & \langle 10|x_1x_2|01\rangle \\ \langle 01|x_1x_2|10\rangle & \langle 01|x_1x_2|01\rangle \end{pmatrix}$$

Now x_1 and x_2 can be expressed in terms of raising and lowering operators as in Problem Sheet 3:

$$x_i \equiv \hat{x}_i = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_i + \hat{a}_i^\dagger)$$

so that

$$x_1x_2 = \frac{\hbar}{2m\omega} \{ \hat{a}_1\hat{a}_2 + \hat{a}_1\hat{a}_2^\dagger + \hat{a}_1^\dagger\hat{a}_2 + \hat{a}_1^\dagger\hat{a}_2^\dagger \}$$

Thus, for example,

$$\langle 10|x_1x_2|01\rangle = \frac{\hbar}{2m\omega} \langle 10| \{ \hat{a}_1\hat{a}_2 + \hat{a}_1\hat{a}_2^\dagger + \hat{a}_1^\dagger\hat{a}_2 + \hat{a}_1^\dagger\hat{a}_2^\dagger \} |01\rangle = \langle 10|\hat{a}_1^\dagger\hat{a}_2|01\rangle = \frac{\hbar}{2m\omega}$$

using the fact that $\hat{a}_1|01\rangle = 0$ to kill the first two terms and the orthogonality properties of the eigenstates to get rid of the fourth term.

By similar arguments, the two diagonal terms in the matrix both vanish whilst $\langle 01|x_1x_2|10\rangle = \langle 10|x_1x_2|01\rangle$.

Thus the 2×2 submatrix of $\Delta\hat{V}$ is $\mathcal{E} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ where $\mathcal{E} \equiv \frac{C\hbar}{2m\omega}$.

The determinant equation for the splittings is thus

$$\begin{vmatrix} -\Delta E & \mathcal{E} \\ \mathcal{E} & -\Delta E \end{vmatrix} = 0$$

which has solutions

$$\Delta E = \pm \mathcal{E}$$

3. 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 diagonal matrix elements for the following perturbations:

- (a) $v\hat{l}_z$
 (b) vr^2
 (c) vr
 (d) $v \exp(-2r/a_0)$
 (e) $v \exp(-Zr/a_0)$

Note: there are a lot of integrals in this question. An important aspect is to “think before you int” - which ones are going to be zero by symmetry?

The first few normalised energy eigenfunctions, $u_{nlm}(\underline{r})$:

$$\begin{aligned} u_{100}(\underline{r}) &= \frac{1}{\sqrt{\pi}}(Z/a_0)^{3/2} \exp(-Zr/a_0) \\ u_{200}(\underline{r}) &= \frac{1}{2\sqrt{2\pi}}(Z/a_0)^{3/2} (1 - Zr/2a_0) \exp(-Zr/2a_0) \\ u_{210}(\underline{r}) &= \frac{1}{4\sqrt{2\pi}}(Z/a_0)^{3/2} (Zr/a_0) \exp(-Zr/2a_0) \cos \theta \\ u_{21\pm 1}(\underline{r}) &= \mp \frac{1}{8\sqrt{\pi}}(Z/a_0)^{3/2} (Zr/a_0) \exp(-Zr/2a_0) \sin \theta \exp(\pm i\phi) \end{aligned}$$

from which, using integration by parts and standard expressions for integrals,

- (a) Remembering that $\hat{l}_z|u_{nlm}\rangle = m\hbar|u_{nlm}\rangle$
 $\langle u_{n'l'}|\hat{l}_z|u_{nlm}\rangle = 0$; ; $\langle u_{211}|\hat{l}_z|u_{211}\rangle = v\hbar$; ; $\langle u_{21-1}|\hat{l}_z|u_{21-1}\rangle = -v\hbar$;
 (b) $\langle u_{100}|vr^2|u_{100}\rangle = 3v(a_0/Z)^2$; ; $\langle u_{200}|vr^2|u_{200}\rangle = 42v(a_0/Z)^2$; ;
 $\langle u_{210}|vr^2|u_{210}\rangle = 30v(a_0/Z)^2$; ; $\langle u_{21\pm 1}|vr^2|u_{21\pm 1}\rangle = 30v(a_0/Z)^2$
 (c) $\langle u_{100}|vr|u_{100}\rangle = 1 \cdot 5v(a_0/Z)$; ; $\langle u_{200}|vr|u_{200}\rangle = 6v(a_0/Z)$; ;
 $\langle u_{210}|vr|u_{210}\rangle = 2 \cdot 5v(a_0/Z)$; ; $\langle u_{21\pm 1}|vr|u_{21\pm 1}\rangle = 2 \cdot 5v(a_0/Z)$
 (d) $\langle u_{100}|ve^{-2r/a_0}|u_{100}\rangle = v(\frac{Z}{Z+1})^3$; ;
 $\langle u_{200}|ve^{-2r/a_0}|u_{200}\rangle = vZ^3[(\frac{1}{Z+2})^3 + (\frac{3Z^2}{(Z+2)^5} + \frac{3Z}{(Z+2)^4})]$; ;
 $\langle u_{21m}|ve^{-2r/a_0}|u_{21m}\rangle = \frac{v}{2}(\frac{Z}{Z+2})^5$;
 (e) $\langle u_{100}|ve^{-Zr/a_0}|u_{100}\rangle = \frac{8v}{27}$; ; $\langle u_{200}|ve^{-Zr/a_0}|u_{200}\rangle = \frac{v}{32}$; ; $\langle u_{21m}|ve^{-Zr/a_0}|u_{21m}\rangle = \frac{v}{64}$

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

Notice that all off-diagonal terms with the same n are zero: none of these perturbations mix the eigenstates. This arises from the orthogonality constraint on the spherical harmonics $\langle Y_{l'm'}|Y_{lm}\rangle = \delta_{l'l'}\delta_{m'm}$. (a) actually commutes with the Hamiltonian, so doesn't mix $n=1$ with $n=2$ states, in this case the energy shifts are exact for any v . (b-e) mix states of $n=1$ and $n=2$, and so perturbation is only correct when the matrix element is much less than the energy difference between the $n=1$ and $n=2$ states ($0.75Z^2$ Ryd.).

4. The change in energy levels in an atom due to the application of an external electric field is known as the Stark effect. The perturbation corresponding to a uniform static electric field of magnitude \mathcal{E} , applied in the z direction to a hydrogen atom is

$$\Delta\hat{V} = e\mathcal{E}z = e\mathcal{E}r \cos\theta$$

Use degenerate perturbation theory to calculate the effect on the 4-fold degenerate $n = 2$ level of atomic hydrogen.

The relevant unperturbed eigenfunctions are:

$$\begin{aligned} u_{200} &= (8\pi a_0^3)^{-1/2} \left(1 - \frac{r}{2a_0}\right) \exp(-r/2a_0) \\ u_{211} &= -(\pi a_0^3)^{-1/2} \frac{r}{8a_0} \sin\theta \exp(i\phi) \exp(-r/2a_0) \\ u_{210} &= (8\pi a_0^3)^{-1/2} \frac{r}{2a_0} \cos\theta \exp(-r/2a_0) \\ u_{21-1} &= (\pi a_0^3)^{-1/2} \frac{r}{8a_0} \sin\theta \exp(-i\phi) \exp(-r/2a_0) \end{aligned}$$

Ignoring spin, we need to calculate the matrix elements of $\Delta\hat{V}$ between the various degenerate $n = 2$ states, giving a 4×4 matrix whose determinant enables us to find the energy shifts to first order. We label the rows and columns of the matrix by the values of the quantum numbers of the various $n = 2$ states, choosing the order 200, 210, 211 and 21 - 1.

We can simplify the calculation by noting that many of the matrix elements

$$\langle 2\ell' m_{\ell'} | \Delta\hat{V} | 2\ell m_{\ell} \rangle = e\mathcal{E} \int \int \int u_{2,\ell',m_{\ell'}}^* (r \cos\theta) u_{2\ell m_{\ell}} r^2 \sin\theta dr d\theta d\phi$$

vanish on symmetry grounds. For example, we note that the perturbation has odd parity ($z \rightarrow -z$ under parity). The eigenfunction u_{200} has even parity, whereas u_{21m} have odd parity. Since the integral over all space of any odd function is zero we have

$$\Delta V_{200,200} = \Delta V_{21m',21m} = 0$$

We also note that

$$\int_0^{2\pi} \exp(\pm i\phi) d\phi = 0$$

and thus

$$\Delta V_{200,211} = \Delta V_{200,21-1} = \Delta V_{211,200} = \Delta V_{21-1,200} = 0$$

Since the perturbation is real, $\Delta V_{200,210} = \Delta V_{210,200}$ and these are the only non-zero matrix elements:

$$\langle 200 | \Delta\hat{V} | 210 \rangle = e\mathcal{E} (8\pi a_0^3)^{-1} \int_0^{2\pi} d\phi \int_0^{\pi} \cos^2\theta \sin\theta d\theta \cdot \frac{1}{2a_0} \int_0^{\infty} r^4 \left(1 - \frac{r}{2a_0}\right) \exp(-r/a_0) dr$$

The ϕ integral is trivial and gives 2π . The θ integral can be written

$$\int_0^{\pi} \cos^2\theta \sin\theta d\theta = \int_{-1}^{+1} \cos^2\theta d(\cos\theta) = \left[\frac{1}{3} \cos^3\theta \right]_{-1}^{+1} = \frac{2}{3}$$

The radial integral is more complicated but can be performed using the result:

$$\int_0^{\infty} \exp(-br) r^n dr = n!/b^{n+1}, \quad n > -1$$

Thus

$$\int_0^{\infty} r^4 \exp(-r/a_0) dr = 4! a_0^5 \quad \text{and} \quad \int_0^{\infty} r^5 \exp(-r/a_0) dr = 5! a_0^6$$

Putting it all together,

$$\langle 200 | \Delta \hat{V} | 210 \rangle = e\mathcal{E} (8\pi a_0^3)^{-1} \times 2\pi \times \frac{2}{3} \times \frac{1}{2a_0} \left[24a_0^5 - \frac{1}{2a_0} 120a_0^6 \right] = -3e\mathcal{E}a_0$$

Thus the determinant equation, with the ordering of rows and columns specified above, is

$$\begin{vmatrix} -\Delta E & -3e\mathcal{E}a_0 & 0 & 0 \\ -3e\mathcal{E}a_0 & -\Delta E & 0 & 0 \\ 0 & 0 & -\Delta E & 0 \\ 0 & 0 & 0 & \Delta E \end{vmatrix} = (\Delta E)^4 - (3e\mathcal{E}a_0)^2(\Delta E)^2 = 0$$

The solutions to this are $\Delta E = \pm 3e\mathcal{E}a_0, 0, 0$. Thus the degeneracy of the eigenfunctions u_{211} and u_{21-1} is not lifted by the perturbation, whereas the u_{200} and u_{210} states are split. The spectral line corresponding to the $n = 2 \rightarrow n = 1$ Lyman α transition is split into three if the hydrogen atom is placed in an electric field.

5. A function has Periodic Boundary Conditions if $\Phi(x) = \Phi(x + L)$ for all x : Why is a particle confined to a 1d ring equivalent to periodic boundary conditions?

Periodic boundary conditions for a function are defined by

$$\Phi(x) = \Phi(x + L)$$

where L is the periodicity

If we set up a coordinate system measuring around a ring of length L , then $x + L$ is the same position in space as x . We have simply gone once around the ring. A particle confined to a ring must have a unique wavefunction everywhere, so the periodic boundary condition criterion holds.

2N non-interacting 'electrons' are confined to a 1d ring of length L. Show that their wavefunctions can be written as

$$\Phi \propto \cos(kx)$$

$$\Phi \propto \sin(kx)$$

and explain what k is. and draw a graph of energy against $k = \frac{2\pi}{\lambda}$. Explain why each state is fourfold degenerate

This is simply equivalent to free particles,

$$\hat{H} = -\hbar^2 \nabla^2 / 2m$$

the wavefunctions are

$$\Phi = \sqrt{\frac{2}{L}} \cos(kx)$$

$$\Phi = \sqrt{\frac{2}{L}} \sin(kx)$$

Where the normalisation constant comes from the mean value of $\cos^2(x)$ over a period being $\frac{1}{2}$. Yes, you should know that!

$$\int_0^L \cos^2(kx) dx = L/2$$

and the energies

$$E_k = \frac{\hbar^2 k^2}{2m}$$

where the wavenumber $k = \frac{2\pi n}{L}$ for any integer quantum number n . The degeneracy arises because there are two possible spin states, and sine and cosine wavefunctions. An alternate way of writing these, with explicit time dependence, is $\Phi = \sqrt{\frac{2}{L}} \exp \pm i(kx - \omega t)$ These can be seen to be waves travelling clockwise and anticlockwise around the ring. Note also that you can add an arbitrary phase angle, defining the value of the wavefunction at the arbitrary origin. Here it is set to zero.

Notice that as L goes to infinity, the gaps in energy between adjacent states go to zero.

Assuming that the electrons occupy the lowest energy states according to the Exclusion Principle, show that the highest energy of an electron is independent of L , provided the electron density N/L is constant

We saw above that $E_k = \frac{\hbar^2 k^2}{2m}$. For Fermions, each electron should have different spin or different k or different sin/cos. Thus states with quantum numbers $n = 1 \dots N/2$ are occupied. The highest allowed value of k is $n = M/2$ i.e. $k = \frac{N\pi}{L}$. This means that the ‘‘Fermi energy’’ does not depend on the size of a sample.

The ions in a 1D solid are represented by a perturbation

$$V(x) = -V_o \cos^2 \pi N x / L$$

Explain why this represents divalent ions.

There are N minima in this potential between 0 and L . Presumably these represent the positions of the ions. Since there are $2N$ electrons, there must be 2 from each ion, implying that the material is divalent.

Show that to first order in perturbation theory, this lowers the energy of the highest energy occupied states by $3v_0/4$ or $v_0/4$

From above, the highest energy occupied spatial state is

$$\Phi = \sqrt{\frac{2}{L}} \cos\left(\frac{\pi N x}{L}\right)$$

so setting $b = \pi Nx/L$

$$\begin{aligned}\Delta E &= -V_o \frac{2}{L} \int_0^L \cos^2(bx) \cos^2(bx) dx \\ &= -\frac{3V_o}{4}\end{aligned}$$

The other highest energy occupied spatial state is

$$\Phi = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi Nx}{L}\right)$$

so

$$\begin{aligned}\Delta E &= -V_o \frac{2}{L} \int_0^L \sin^2(bx) \cos^2(bx) dx \\ &= -\frac{V_o}{4}\end{aligned}$$

Note that the average value of the perturbing potential is $-\frac{V_o}{2}$, the same as the average of these two states. One moves up in energy, the other moves down.

Explain how this perturbation affects conductivity

Without the perturbation, for large N there are degenerate electron levels at the Fermi surface, thus the energy cost to move an electron from a clockwise state to an anticlockwise state is infinitesimally small. With the perturbation, it costs finite energy to raise the electron from the highest occupied state to the lowest unoccupied state, so a small electric field produces no current. If the gap ($V_o/2$) is small enough, some electrons will be thermally excited into the high energy band: the material is a semiconductor.

You may use the results that for any integer N

$$\begin{aligned}\int_0^L \cos^4(N\pi x/L) dx &= 3L/8 \\ \int_0^L \cos^2(N\pi x/L) \sin^2(N\pi x/L) dx &= L/8\end{aligned}$$

6. This question was removed from the 2009/10 tutorial sheet

Consider the proton in a hydrogen atom to be a uniform sphere of charge, of radius $R \ll a_0$, rather than a point charge. What is the classical electrostatic potential energy function, $V(r)$, of the electron? [Hint: use Gauss's Law to find the internal and external electric fields and hence the electrostatic potential, $\Phi(r)$. Remember that the corresponding potential energy is $-e\Phi(r)$]

An exercise in electrostatics! For $r < R$, consider a spherical Gauss surface of radius r as shown in the figure. The total charge Q enclosed is

$$Q = \frac{4}{3}\pi r^3 \rho \quad \text{where} \quad \rho = \frac{3e}{4\pi R^3}$$

By symmetry, the electric field, $\underline{\mathcal{E}}$ is purely radial and so the flux through the Gaussian surface is $\mathcal{E} \times 4\pi r^2$. Gauss' Law

$$\int_S \underline{\mathcal{E}} \cdot \underline{dS} = \frac{Q}{\epsilon_0}$$

then tells us that

$$4\pi r^2 \mathcal{E} = \frac{Q}{\epsilon_0} = \frac{e}{\epsilon_0} \cdot \left(\frac{r}{R}\right)^3$$

Thus

$$\mathcal{E} = \frac{er}{(4\pi\epsilon_0)R^3} = -\frac{d\Phi(r)}{dr} \quad \text{giving} \quad \Phi(r) = \frac{e}{(4\pi\epsilon_0)R^3} \left[-\frac{1}{2}r^2\right] + c$$

where $\Phi(r)$ is the electrostatic potential and c is a constant of integration.

For $r > R$, the electric field is the same as for a point charge, e , at the origin and so

$$\Phi(r) = \frac{e}{(4\pi\epsilon_0)r}, \quad r > R$$

We can fix the constant, c , by matching the interior and exterior solutions for Φ at the surface of the proton, $r = R$:

$$\Phi(R) = \frac{e}{(4\pi\epsilon_0)R^3} \left[-\frac{1}{2}R^2\right] + c = \frac{e}{(4\pi\epsilon_0)R} \quad \text{giving} \quad c = \frac{3e}{8\pi\epsilon_0 R}$$

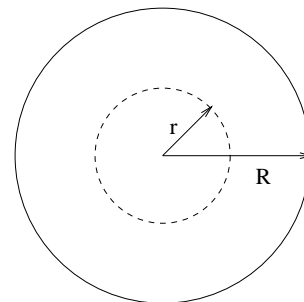
The electrostatic potential energy for an electron of charge $-e$ in the potential $\Phi(r)$ is thus

$$V(r) = -e\Phi(r) = \begin{cases} -\frac{3e^2}{8\pi\epsilon_0 R^3} \left[R^2 - \frac{r^2}{3}\right], & r < R \\ -\frac{e^2}{4\pi\epsilon_0 r}, & r > R \end{cases}$$

By treating the difference between the electrostatic potential energy of the electron in the field of such a finite-size proton and in the field of a point proton by perturbation theory, find the shift in the ground-state energy of the hydrogen atom arising from the finite size of the proton. Estimate the order of magnitude of this shift, given that $R \simeq 10^{-15} \text{ m}$.

The perturbation is

$$\Delta \hat{V} = \begin{cases} -\frac{3e^2}{8\pi\epsilon_0 R^3} \left[R^2 - \frac{r^2}{3}\right] + \frac{e^2}{4\pi\epsilon_0 r}, & r < R \\ 0, & r > R \end{cases}$$



The unperturbed ground-state wavefunction for hydrogen is

$$u_{100}(r) = (\pi a_0^3)^{-1/2} \exp(-r/a_0)$$

so the energy shift is

$$\Delta E = \langle 100 | \Delta \hat{V} | 100 \rangle = \frac{4\pi}{\pi a_0^3} \int_0^R \Delta V(r) \exp(-2r/a_0) r^2 dr$$

Since $R \ll a_0$, we can put $\exp(-2r/a_0) = 1$, giving

$$\begin{aligned} \Delta E &= \frac{4}{a_0^3} \frac{e^2}{2(4\pi\epsilon_0)} \left\{ -3 \left(\frac{1}{R} \left[\frac{r^3}{3} \right]_0^R - \frac{1}{3R^3} \left[\frac{r^5}{5} \right]_0^R \right) + \left(2 \left[\frac{r^2}{2} \right]_0^R \right) \right\} \\ &= \frac{4}{5} \left(\frac{R}{a_0} \right)^2 \cdot \frac{e^2}{2(4\pi\epsilon_0)a_0} = \frac{4}{5} \left(\frac{R}{a_0} \right)^2 \text{ Ry} \end{aligned}$$

Now $a_0 = 0.53 \times 10^{-10}$ m and $R \simeq 10^{-15}$ m and thus $\Delta E \simeq 2.85 \times 10^{-10}$ Ry or 3.87×10^{-9} eV, an extremely small effect!