1. The Deuteron. A deuteron (^{2}H nucleus) is a bound state of a neutron (charge 0, mass 939.5 MeV) and a proton (charge e, mass 938.2 MeV). Scattering measurements determine that the separation of the neutron and proton is about $a = 1.5$ fm and the binding energy, determined from mass measurements, is $E_b = 2.226$ MeV. Approximate the potential energy as a spherical square well, $V(r) = -V_0$ for $r < a$ and $V(r) = 0$ for $r > a$.

(a) What is the value of V_0 in MeV?

Solution

Using separation of variables, we arrive at the radial equation (as in lecture),

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right) R(r) = -E_b R(r)\,,$$

where l is the angular momentum quantum number and $m = 469.4$ MeV is the reduced mass of the proton and neutron. We let $R(r) = u(r)/r$, so $u(r \to 0) \propto r^{(l+1)}$, and the equation becomes (again, as in lecture),

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right) u(r) = -E_b u(r)\,.$$

The ground state will occur for $l = 0$. We let

$$\kappa = \sqrt{\frac{2mE_b}{\hbar^2}} \qquad k = \sqrt{\frac{2m(V_0 - E_b)}{\hbar^2}}\,,$$

Then for $r < a$, $u(r) = \sin(kr)$ to satisfy the boundary condition at $r = 0$, and for $r > a$, $u(r) = A\exp(-\kappa r)$ to produce a normalizable function. We match u and it's derivative at a which yields

$$ka \cot ka = -\kappa a\,.$$

The right hand side of this equation is (use $\hbar = 6.5817 \times 10^{-16}$ eV s) is $-\kappa a = -0.3471$. This yields $ka = 1.765$ or $k = 1.177 \times 10^{13}\,\mathrm{cm}^{-1}$and

$$V_0 = \frac{\hbar^2 k^2}{2m} + E_b = 59.7\,\mathrm{MeV}\,.$$

End Solution

(b) Can the deuteron have an excited (but still bound!) state with $l = 0$?

Solution

The largest energy for any excited state is 0. Assuming this energy, then $\kappa_e = 0$ (the subscript e denotes excited!) and the condition on k_e becomes $k_e a \cot k_e a = 0$. But $k_e a > ka$, so the smallest possible value of $k_e a$ is $k_e a = 3\pi/2$. This gives

$$\frac{\hbar^2 k_e^2}{2m} = 409.9\,\mathrm{MeV} > V_0\,.$$

This is inconsistent with a bound state (the kinetic energy in the well should be less than the well depth), so there can be no excited states with $l = 0$.

End Solution

(c) What do you think about bound states with $l > 0$? (An elaborate calculation is not required!)

Solution

Bound states with $l > 0$ don't exist either. There's just no room for them in the 2.226 MeV between the level of the ground state and the top of the well. The easiest way to see this is to note that

$$\frac{\hbar^2 l(l+1)}{2mr^2} \gtrsim \frac{2\hbar^2}{2ma^2} = 37\,\text{MeV} .$$

End Solution

2. This problem appeared on the January, 2002 prelims. Unless I'm missing something, the condition asked for is a transcendental equation involving U_0.

A particle of mass m moves in the spherically symmetrical potential in 3 dimensions:

$$V(r) = \begin{cases} 0, & 0 \le r < a, \\ -U_0, & a < r < b, \\ 0, & b < r, \end{cases}$$

where $U_0 > 0$.

What is the condition on U_0 so that there will not be any bound states?

Solution

Suppose there is a bound state with energy $-E_b$. Then for $r < a$ and $r > b$, solving the radial Schroedinger equation:

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) \right) u(r) = -E_b u(r) ,$$

with $l = 0$ and where $u(r) = rR(r)$ and $R(r)$ is the radial wave function, gives $u(r) = \exp(\pm\kappa r)$ where $\kappa = \sqrt{2mE_b/\hbar^2}$. For $r < a$, the solution is $A \sinh \kappa r$ in order that it vanish at $r = 0$ to satisfy the boundary condition there. For $r > b$, the solution is $B \exp(-\kappa r)$ in order that we have a normalizable solution. For $a < r < b$, the solution is

$$u(r) = \cos(kr - \phi) ,$$

where $k = \sqrt{2m(U_0 - E_b)/\hbar^2}$ and where ϕ is supposed to be between kb and ka.

So the wave function (actually $u(r)$) starts at 0 at $r = 0$ and grows ($\sinh \kappa r$) to $r = a$ where it attaches to the cosine function which curves back towards the axis and attaches to the exponentially decaying function at $r = b$. If we are looking for the ground state, the cosine cannot cross 0 between a and b. If it did, then it corresponds to an excited state. Thus $kb - ka < \pi$. Matching u and its derivative at both a and b yields the following

$$A \sinh \kappa a = \cos(ka - \phi) \qquad \cos(kb - \phi) = Be^{-\kappa b} \; ,$$
$$\kappa A \cosh \kappa a = -k \sin(ka - \phi) \qquad - k \sin(kb - \phi) = -\kappa B e^{-\kappa b} \; .$$

We can take the ratio of these conditions to cancel out A and B,

$$-k \tan(ka - \phi) = \kappa \coth \kappa a \qquad k \tan(kb - \phi) = -\kappa \; .$$

Now, if we make U_0 smaller so it's approaching the limit where the bound state disappears, then $\kappa \to 0$. From the second of the two equations above, we see that $\tan(kb - \phi) \to 0$ which means $\phi = kb - n\pi$ for some integer n. From the first of the equations above, we have

$$-k \tan(ka - \phi) \to \frac{\kappa}{\kappa a} = \frac{1}{a} \; ,$$

and plugging in the result for kb, we have

$$ka \tan(kb - ka - n\pi) = ka \tan(kb - ka) = 1 \; ,$$

This, together with

$$k = \sqrt{\frac{2mU_0}{\hbar^2}} \; ,$$

and the constraint that $kb - ka < \pi$ provides the condition on U_0 which we could solve given a, b, and m.

If we let $a \to 0$, then we have a square well surrounding the origin as was postulated for the deuteron in problem 1. In this case, the solution of the transcendental equation is $kb = \pi/2 = 1.571$. If you solved problem 1, you came up with $ka = 1.765$, just a little bigger than $\pi/2$, and of course, the deuteron is just barely bound!

———————— End Solution ————————

3. Hydrogen. For the H atom ground state wave function, compute the following expectation values.

$$\left\langle \frac{e^2}{r} \right\rangle , \quad \left\langle \frac{p^2}{2m} \right\rangle , \quad \langle r \rangle \; , \quad \langle p_r \rangle \; , \quad \langle x \rangle \; , \quad \langle p_x \rangle \; , \quad \Delta r \Delta p_r \; , \quad \Delta x \Delta p_x \; .$$

Recall, the wave function is

$$\psi(r, \theta, \phi) = \frac{1}{\sqrt{2}} \left(\frac{2}{a} \right)^{3/2} e^{-r/a} \frac{1}{\sqrt{4\pi}} \; ,$$

where $a = \hbar^2/me^2$ and m is the reduced mass of the electron and proton.

Solution

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{2}\left(\frac{2}{a}\right)^3 \int_0^\infty e^{-2r/a}\,\frac{1}{r}\,r^2 dr = \frac{1}{a}\int_0^\infty e^{-x}x\,dx = \frac{1}{a}\,,$$

so $\langle e^2/r \rangle = e^2/a$. This means the expectation value of the potential energy is $-e^2/a$. The total energy is $-e^2/2a$, and the kinetic energy is the difference, $\langle p^2/2m \rangle = e^2/2a$.

$$\langle r \rangle = \frac{1}{2}\left(\frac{2}{a}\right)^3 \int_0^\infty e^{-2r/a}\,r\,r^2 dr = \frac{1}{2}\frac{a}{2}\int_0^\infty e^{-x}x^3\,dx = \frac{a}{4}3! = \frac{3a}{2}\,.$$

$\langle p_r \rangle = 0$. Recall,

$$p_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\,.$$

We've already shown that $\langle 1/r \rangle = 1/a$. The derivative with respect to r when operating on $\exp(-r/a)$ brings down a $-1/a$ which cancels the $1/a$ from the other term.

$\langle x \rangle = \langle p_x \rangle = 0$ by symmetry. (Or, masochists can calculate $\langle r \sin\theta\cos\phi \rangle$ and since there's no angular dependence in the wave function, the angular terms will integrate to zero.)

For Δr we need to calculate $\langle r^2 \rangle$.

$$\langle r^2 \rangle = \frac{1}{2}\left(\frac{2}{a}\right)^3 \int_0^\infty e^{-2r/a}\,r^2\,r^2 dr = \frac{1}{2}\left(\frac{a}{2}\right)\int_0^\infty e^{-x}x^4\,dx = \frac{a^2}{8}4! = 3a^2\,.$$

So, $\Delta r = \sqrt{3}a/2$. For the ground state, $\langle p_r^2 \rangle = \langle p^2 \rangle = 2m(e^2/2a) = me^2/a = \hbar^2/a^2$. So $\Delta p_r = \hbar/a$ and $\Delta r \Delta p_r = \sqrt{3}\,\hbar/2$.

By symmetry, $\langle x^2 \rangle = \langle r^2 \rangle/3 = a^2$, so $\Delta x = a$. Similarly, $\langle p_x^2 \rangle = \langle p_r^2 \rangle/3 = \hbar^2/3a^2$ and $\Delta p_x = \hbar/\sqrt{3}\,a$. So, $\Delta x \Delta p_x = \hbar/\sqrt{3}$.

End Solution

4. An electron outside liquid Helium. Based on a problem from Schwabl. The region $x < 0$ is filled with liquid helium and $x > 0$ is a vacuum. (Well, we have to ignore the vapor pressure of the helium!) An electron is at $x > 0$ and its potential energy is approximately described by $V(x) = +\infty$ for $x < 0$, due to the repulsion of the electron from the surface, and $V(x) = -Ze^2/x$ for $x > 0$ due to the image charge below the surface. $Z = (\epsilon - 1)/4(\epsilon + 1)$ where ϵ is the dielectric constant and for He, $\epsilon = 1.057$. The motion parallel to the surface is just that of a free particle, so we are only concerned with the motion perpendicular to the surface.

(a) Obtain expressions for the (bound state) energy eigenvalues and eigenfunctions.

Solution

The time independent Schroedinger equation for $x > 0$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{Ze^2}{x}\right)u(x) = Eu(x)\,,$$

where $u(x)$ is the wave function which must vanish at $x = 0$ due to the infinite step in potential there. This equation is just like that for the radial wave function of the Hydrogen atom (after making the substitution $u(r) = rR(r)$) for s-states ($l = 0$). We solve the equation in the same way! We note that for $x \to 0$, the leading term in $u(x)$ must be x. For $x \to \infty$, $u(x) \to \exp(-\kappa x)$, where $\kappa = \sqrt{-2mE/\hbar^2}$. We let $\rho = \kappa x$, and $u(\rho) = \rho \exp(-\rho) w(\rho)$. We let $\rho_0 = Ze^2\kappa/(-E)$. The equation becomes,

$$\rho\frac{d^2 w}{d\rho^2} + 2(1-\rho)\frac{dw}{d\rho} + (\rho_0 - 2)w = 0\,.$$

This is the same as the equation we arrived at when solving the hydrogen atom, except $l = 0$. If we try to solve with a power series, we will get a one term recursion relation. We will also find that the series asymptotically approaches $\exp(+2\rho)$ unless it terminates. The requirement that it terminate means that

$$\rho_0 = 2(N+1)\,,$$

where $N = 0, 1, 2, 3, \ldots$ and w is an N^{th} order polynomial in ρ. Furthermore, using the definition of ρ_0 above, we find

$$E_N = -\frac{mZ^2e^4}{2\hbar^2(N+1)^2} = -\frac{Ze^2}{a(N+1)^2}\,,$$

where a is similar to the Bohr radius,

$$a = \frac{\hbar^2}{mZe^2}\,.$$

So far, we've learned the energy eigenvalues and we also have (although we didn't write it down) a recursion relation for the coefficients of the polynomial $w(\rho)$. So the problem is essentially solved. However, we should write the normalized eigenfunctions in terms of standard functions. We do this the same way as for the hydrogen radial eigenfunctions. $w(\rho)$ turns out to be an associated Laguerre polynomial in 2ρ. Recall

$$L_n^p(z) = \sum_{m=0}^{n} (-1)^m \frac{((n+p)!)^2}{(n-m)!(p+m)!m!} z^m \,.$$

The polynomials we used for the hydrogen atom were L_{n-l-1}^{2l+1} with $n = N + l + 1$. So, the solutions here will involve $L_N^1(2\rho)$. Pulling everything together,

$$u_N(x) = \left(\frac{2}{a(N+1)} \frac{N!}{2(N+1)[(N+1)!]^3}\right)^{1/2} e^{-x/a(N+1)} \frac{2x}{a(N+1)} L_N^1\left(\frac{2x}{a(N+1)}\right) \,.$$

——— End Solution ———

(b) What is the numerical value of the ground state energy?

——— Solution ———

The expression for E_0 is the same as for the ground state of the hydrogen atom. The difference is that here, Z depends on the dielectric constant of liquid helium, not the number of charges in the nucleus. Using the given dielectric constant, $Z = 0.00693$, so it's a weak charge attracting the electron. The energy is proportional to Z^2, so with $-13.6\,\mathrm{eV}$ for the ground state energy of hydrogen, we find $E_0 = -0.65\,\mathrm{meV}$. Also, as a point of interest, the parameter a here is $1/Z = 144$ times the Bohr radius or about $76\,\text{Å}$.

——— End Solution ———

(c) Explicitly list the first four eigenfunctions. Be sure they are normalized.

——— Solution ———

$$u_0(x) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{a}}\, e^{-x/a} \frac{2x}{a} \,.$$

$$u_1(x) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{2a}}\, e^{-x/2a} \frac{2x}{2a} \left(1 - \frac{1}{2}\frac{2x}{2a}\right) \,.$$

$$u_2(x) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{3a}}\, e^{-x/3a} \frac{2x}{3a} \left(1 - \frac{2x}{3a} + \frac{1}{6}\left(\frac{2x}{3a}\right)^2\right) \,.$$

$$u_3(x) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{4a}}\, e^{-x/4a} \frac{2x}{4a} \left(1 - \frac{3}{2}\frac{2x}{4a} + \frac{1}{2}\left(\frac{2x}{4a}\right)^2 - \frac{1}{24}\left(\frac{2x}{4a}\right)^3\right) \,.$$

——— End Solution ———