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HOMEWORK #6#

Course 314,Introduction In Quantum Mechanics,Professor K. Griffioen

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1 Problem 7.1

Use the gausian trial function (Equation 7.2) to obtain the lowest upper bound you can on the ground-state energy of (a) the linear potential : $V(x) = \alpha|x|$; (b) the quartic potential : $V(x) = \alpha x^4$.

2 Solution

(a) The gaussian trial wavefunction is given by :

$$\psi(x) = Ne^{-bx^2} \tag{1}$$

where N is the normalization constant: $N = (\frac{2b}{\pi})^{1/4}$,so the normalized wavefunction has the following form :

$$\psi(x) = (\frac{2b}{\pi})^{1/4} e^{-bx^2} \tag{2}$$

The energy eigenstate is given by the average of H, $< H >$, where the Hamiltonian is given by :

$$H = -\frac{\hbar}{2m}\frac{d}{dx^2} + \alpha|x| \tag{3}$$

The average $< H >$ by definition is given as :

$$< H > = \frac{< \psi(x)|H|\psi(x) >}{< \psi(x)|\psi(x) >} \tag{4}$$

We'll have then :

$$E = < H > = \int_{-\infty}^{+\infty} dx \psi(x) H \psi(x)^* \tag{5}$$

$$
\begin{aligned}
E =< H >= & \quad (\frac{2b}{\pi})^{1/2} \int_{-\infty}^{+\infty} dx e^{-bx^2} \left(-\frac{\hbar}{2m}\frac{d}{dx^2} + \alpha|x| \right) e^{-bx^2} \\
E =< H >= & \quad (\frac{2b}{\pi})^{1/2} \int_{-\infty}^{+\infty} dx \left[\frac{\hbar b}{m}(1-2bx^2)e^{-2bx^2} + \alpha|x|e^{-2bx^2} \right] \\
E =< H >= & \quad \frac{hbar^2}{2m} + \frac{\alpha}{\sqrt{2\pi b}}
\end{aligned}
$$

To find the lowest upper bound on eigenenergy of the ground state we'll minimize the $< H >$ with respect of b :

$$
\begin{aligned}
\frac{d < H >}{dx} = & \quad \frac{\hbar}{2m} - \frac{\alpha}{\sqrt{2\pi}} b^{-3/2} = 0, \\
b = & \quad \left(\frac{m\alpha}{\hbar^2\sqrt{2\pi}} \right)^{2/3}
\end{aligned}
\tag{6}
$$

Substituting into $< H >$ expression we'll find the minimum of energy :

$$
E_{min} =< H >_{min} = \frac{3m}{2} \left(\frac{\hbar\alpha}{m^2\sqrt{2\pi}} \right)^{2/3}
\tag{7}
$$

(b) For The quartic potential $V(x) = \alpha x^4$ we'll do the same steps and we'll find that :

$$
\begin{aligned}
< H >= & \quad \frac{\hbar^2 b}{2m} + \alpha \left(\frac{2b}{\pi} \right)^{1/2} \int_{-\infty}^{+\infty} x^4 e^{-2bx^2} dx \\
< H >= & \quad \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}
\end{aligned}
\tag{8}
$$

We'll minimize the above expression and we'll find the minimum average of the Hamiltonian $< H >$:

$$
\begin{aligned}
\frac{d < H >}{db} = & \quad \frac{\hbar}{2m} - \frac{3\alpha}{8b^3} = 0 \\
b = & \quad \left(\frac{3\alpha m}{4h^2} \right)^{1/3}
\end{aligned}
\tag{9}
$$

Than, like before, we'll plug the b into $< H >$ and we'll find the E_{min} :

$$E_{min} =< H >_{min}= \frac{9}{8}\left(\frac{3\alpha m}{4\hbar^2}\right)^{-2/3} \tag{10}$$

3 Problem 7.7

Apply the tehniques of this Section to the H^- and H^+ ions (each has two electrons, like helium, but nuclear charges $Z = 1$ and $Z = 3$, respectively). Find the effective (partially shielded) nuclear charge, and determine the best upper bound on 4 E$_g$, for each case. *Note*: In the case of H^- you should find that $< H > > -13,6eV$, which would appear to indicate that there is no bound state at all, since it is energetically favorable for one electron to fly off, leaving behind a neutral hydrogen atom.This is not entirely surprising, since the electrons are less strongly attractedto the nucleus than they are in helium, and the electron repulsion tends to break the atom apart. However, it turns out to be incorrect. With a more sophisticated trial wave function (see Problem7.16) it can be shownthat $E_g < -13.6eV$, and hence that a bound state does exist. It's only *barely* bound, however, and there are no excited bound states, so H^- has no discrete spectrum (all transitions are to and from the continuum). As a result, it is difficult to study in the laboratory, although it exists in great abundance on the surface of the sun.

4 Solution

The trial wave function has the following form :

$$\psi(r_1, r_2) = \frac{z^3}{\pi a^3} e^{-Z(r_1+r_2)/a} \tag{11}$$

Then the Hamiltonian is given by :

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{Z}{r_1} + \frac{Z}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0}\left(\frac{(Z-1)}{r_1} + \frac{(Z-1)}{r_2} + \frac{1}{|r_1 - r_2|}\right) \tag{12}$$

The expectation value of H will be :

$$< H >= 2Z^2E_1 + 2(Z-1)\left(\frac{e^2}{4\pi\epsilon_0}\right) < \frac{1}{r} > + < V_{ee} > \tag{13}$$

The expectation value of V_{ee} for an arbitrary Z will be :

$$V_{ee} = \frac{5Z}{8a}\left(\frac{e^2}{4\pi\epsilon_0}\right) = -\frac{5Z}{4}E_1 \tag{14}$$

From (13) and (14) we'll get the $< H >$:

$$\begin{aligned} < H >= & \left[2Z^2 - 4Z(Z-1) - (5/4)Z\right]E_1 \\ < H >= & \left[-2Z^2 + (11/4)Z\right]E_1 \end{aligned} \tag{15}$$

The lowest upper bound occurs when $< H >$ is minimized :

$$\begin{aligned} \frac{d}{dZ} < H >= & \left[-4Z + (11/4)\right]E_1 = 0, \\ Z = & \frac{11}{16} = 0.687 \end{aligned} \tag{16}$$

We'll plug the value of Z in (15),and we'll find for H^- :

$$< H >= \frac{11}{16}\left[-2(\frac{11}{16}) + (\frac{11}{4})\right]E_1 = -2\left(\frac{11}{16}\right)^2 E_1 = -12.87eV \tag{17}$$

where Bohr energy $E_1 = -13.6eV$.

For Li^+ with $Z = 3$ the expectation value of H will be :

$$\begin{aligned} < H >= & \left[2Z^2 - 4Z(Z-3) - (5/4)Z\right]E_1, \\ < H >= & \left[-2Z^2 + (43/4)Z\right]E_1 \end{aligned} \tag{18}$$

The lowest upper bound is given by minimum of $< H >$:

$$\begin{aligned} \frac{d}{dZ} < H >= & \left[-4Z + (43/4)\right]E_1 = 0, \\ Z = & \frac{43}{16} = 2.68 \end{aligned} \tag{19}$$

The minimum expectation value of H will be than :

$$< H >_{min} = 2Z^2 E_1 = -195.2 eV \tag{20}$$

5 Problem 7.12

If the photon had a nonzero mass ($m_\gamma \neq 0$), the Coulomb potential would be replaced by a **Yukawa potential** , of the form

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r} \tag{21}$$

where $\mu = m_\gamma c/\hbar$. With a trial wave function of your own devising, estimate the binding energy of a " hydrogen" atom with this potential. Assume $\mu a << 1$, and give your answer correct to order $(\mu a)^2$.

6 Solution

The perturbed Hamiltonian will be :

$$H = -\frac{\hbar^2}{2m}\nabla^2 \ - \frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r} \tag{22}$$

We'll choose the hidrogen-like trial wave function $\psi = Ae^{-br}$, where the normalization constant is given by $A = \left(\frac{1}{\pi a^3}\right)^{1/2}$.In this case $b = -1/a$.Then the wave function will be :

$$\psi(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \tag{23}$$

The expectation value of H is equal with the sum of expectation values of kinetic energy $< T >$ and potential energy $< V >$:

$$< H > = < T > + < V > \tag{24}$$

By definition the expectation value of an observable H is give by :

$$< H > = \frac{< \psi|H|\psi >}{< \psi|\psi >}, \tag{25}$$

The expectation value of the potential energy will be :

$$<V>= \quad -\frac{e^2}{4\pi^2\epsilon_0 a^3}\int_0^{2\pi} d\phi \int_0^{\pi} sin\theta d\theta \int_0^{\infty} re^{-(\mu+2/a)r}dr, \tag{26}$$
$$<V>= \quad -\frac{e^2}{\pi a^3\epsilon_0}\int_0^{\infty} re^{-(\mu+2/a)r}dr,$$
$$<V>= \quad -\frac{e^2}{\pi a^3\epsilon_0}\frac{1}{(\mu+2/a)^2}$$

The expectation value of the kinetic energy will be :

$$\nabla^2\psi = \quad \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) = \frac{1}{\sqrt{\pi a^3}}\left(\frac{1}{a^2}-\frac{2}{ra}\right)e^{-2r/a}, \tag{27}$$
$$<T>= \quad -\frac{\hbar^2}{2m}\int_0^{2\pi} d\phi \int_0^{\pi} sin\theta d\theta \int_0^{\infty}\frac{1}{\pi a^4}\left(\frac{r^2}{a}-2r\right)e^{-2r/a}dr,$$
$$<T>= \quad \frac{4\hbar^2}{ma^4}\int_0^{\infty} re^{-2r/a}dr - \frac{2\hbar^2}{ma^5}\int_0^{\infty} r^2e^{-2r/a}dr,$$
$$<T>= \quad \frac{4\hbar^2}{ma^4}\left(\frac{a^2}{4}\right)-\frac{2\hbar^2}{ma^5}\left(\frac{a^3}{4}\right),$$
$$<T>= \quad \frac{\hbar^2}{2ma^2}$$

We'll plug (26) and (27) in (24) and we'll obtain :

$$<H>= \frac{\hbar^2}{2ma^2}-\frac{e^2}{\pi a^3\epsilon_0}\frac{1}{(\mu+2/a)^2} \tag{28}$$

Assuming that $\mu a << 1$, we can expand $(1+\mu a/2)^{-2}$ in Taylor series :

$$(1+\mu a/2)^{-2} = \quad 1-2\left(\frac{\mu a}{2}\right)+3\left(\frac{\mu a}{2}\right)^2, \tag{29}$$
$$(1+\mu a/2)^{-2} = \quad 1-\mu a+\frac{3}{4}(\mu a)^2$$

The expectation value of H becomes :

$$<H>= \quad \frac{\hbar^2}{2ma^2}-\frac{e^2}{4\pi a\epsilon_0}\left[1-(\mu a)+\frac{3}{4}(\mu a)^2\right], \tag{30}$$

$$< H >= \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi a\epsilon_0} + \frac{\mu e^2}{4\pi\epsilon_0} - \frac{3(e\mu)^2}{4\pi\epsilon_0}a$$

The binding energy up to order $(\mu a)^2$ is given exactly by the relation (30).

7 Problem 8.1

Use the WKB approximation to find the allowed energies (E_n) of an infinite square well with a "shelf", of height V_0, extending half-way across (see Figure 6.3) :

$$\begin{cases} V_0, & \text{if } 0 < x < a/2, \\ 0, & \text{if } a/2 < x < a, \\ \infty, & \text{otherwise.} \end{cases} \tag{31}$$

Express your answer in terms of V_0 and $E_n^0 \equiv (n\pi\hbar)/2ma^2$(the nth allowed energy for the "unperturbed" infinite square well, with *no* shelf). Assume that $E_1^0 > V_0$, but do *not* assume that $E_n >> V_o$. Compare your result with what we got in Section 6.1.2, using first-order perturbation theory. note that they are in agreement if either V_0 is very small (the perturbation theory regime) or n is very large (the semiclassical WKB regime).

8 Solution

WKB approximation gives us that :

$$\begin{aligned} n\pi\hbar &= \int_0^a p(x)dx, \qquad (32) \\ n\pi\hbar &= \int_0^{a/2} \sqrt{2m(E-V_0)}dx + \int_{a/2}^a \sqrt{2mE}, \\ \frac{2n\pi\hbar}{a\sqrt{2m}} &= \sqrt{E-V_0} + \sqrt{E}, \\ \frac{2n^2\pi^2\hbar^2}{a^2m} &= 2E - V_0 + 2\sqrt{E(E-V_0)}, \end{aligned}$$

We'll substitute the $\beta = \frac{2n^2\pi^2\hbar^2}{a^2m}$, and then the expression will become :

$$(\beta + V_0 - 2E)^2 = 4E^2 - 4EV_0, \tag{33}$$

$$E = \frac{(\beta + V_0)^2}{4\beta}$$

If $V_0 << \beta$ then :

$$E = \frac{\beta}{4} + \frac{V_0}{2} = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{34}$$

which is the same result as on page 224.

9 Problem 8.3

Use Equation 8.22 to calculate the approximate transmission probability for a particle of energy E that encounters a finite square barrier of height $V_0 > E$ and width $2a$. Compare the exact result (Prob. 2.32) in the WKB regime $T << 1$.

10 Solution

The equation 8.22 gives us that :

$$\begin{aligned} T &= e^{-2\gamma}, \\ \gamma &= \frac{1}{\hbar}\int_0^{2a} |p(x)|dx, \\ |p(x)| &= \sqrt{2m(V_0 - E)} \end{aligned} \tag{35}$$

Then the transmission probability for a particle of energy E will be :

$$T = E^{-\frac{4a}{\hbar}\sqrt{2m(V_0-E)}} \tag{36}$$

From the result of problem 2.32 we have that :

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right) \tag{37}$$

In the limit $T^{-1} >> 1$ we can approximate the function $(sinhx)^2$ as follows :

$$sinh^2 x = \left(\frac{e^x - e^{-x}}{2}\right)^2 = \frac{e^{2x}}{4} \tag{38}$$

In our case $x = \frac{2a}{\hbar}\sqrt{2m(V_0 - E)}$, and if we'll plug into (37), we'll obtain :

$$T^{-1} = \frac{V_0^2}{16E(V_0 - E)} e^{\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}} \tag{39}$$

The exponents agree in both approximations.The factors in front are the same when $V_0 \approx 15E$.

References

[1] D. J. Griffiths, Introduction To Quantum Mechanics, 1995