TFY4205 Quantum Mechanics II
Problemset 3 fall 2022

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SUGGESTED SOLUTION

Problem 1
The deviation takes the form

$$\lambda H_1 = \begin{cases} \frac{Ze^2}{4\pi\varepsilon_0}\left(\frac{1}{r} - \frac{3}{2R} + \frac{r^2}{2R^3}\right) \text{ for } r \leq R \\ 0 \text{ for } r > R. \end{cases} \tag{1}$$

The contribution in first order perturbation theory is the same as the expectation value of the perturbation in the unperturbed state:

$$\langle 0|\lambda H_1|0\rangle = \int \lambda H_1(r)(\psi_{100})^2 d^3r. \tag{2}$$

The integrand is spherically symmetric and using standard techniques we arrive at

$$\langle 0|\lambda H_1|0\rangle = \frac{R^2}{a^2}\frac{Ze^2}{10\pi\varepsilon_0 a}. \tag{3}$$

The total result for the energy eigenvalue is then

$$E_1 = E_1^0\left(1 - \frac{4}{5}\frac{R^2}{a^2}\right). \tag{4}$$

Since $R/a \ll 1$, this correction is very small (magnitude 10^{-9} eV). Since E_1^0 is negative, the correction will increase the ground state energy. This is reasonable since the perturbation increases the Coulomb potential for $r < R$. For larger Z, the correction will be more important due to the finite size of the nucleus, since $E_1^0 \propto Z^2$, $a^{-2} = Z^2/a_0^2$, and because R is larger. Again, this is physically reasonable since the larger the nuclear charge, the closer the electron will be attracted to the nucleus, where it feels the deviation from a pure Coulomb potential.

Problem 2
According to the variational method, an upper estimate for the ground state energy is

$$E[f] = \frac{\int_{-\infty}^{\infty} f^*(x)\hat{H}f(x)dx}{\int_{-\infty}^{\infty} f^*(x)f(x)dx}. \tag{5}$$

Since our trial functions satisfy $f(\pm\infty) = 0$, we have

$$-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} f^*\frac{d^2f}{dx^2}dx = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{df^*}{dx}\frac{df}{dx}dx. \tag{6}$$

The trial functions are real, meaning that we can compute

$$E[f] = \frac{\int_{-\infty}^{\infty}[\frac{\hbar^2}{2m}(f')^2 + V(x)f^2]dx}{\int_{-\infty}^{\infty} f^2 dx}. \tag{7}$$

For $f(x) = \mathrm{e}^{-\lambda x^2}$, we find that

$$E[f] = \frac{\frac{\hbar^2}{2m}\sqrt{\frac{\pi\lambda}{2}} - \alpha}{\sqrt{\frac{\pi}{2\lambda}}}. \tag{8}$$

The minimum of this functional can be found by differentiating with respect to λ or by rewriting the expression. Using the latter procedure, we see that $E[f]$ can be written as

$$E[f] = \Big(\sqrt{\frac{\hbar^2\lambda}{2m}} - \alpha\sqrt{\frac{m}{\pi\hbar^2}}\Big)^2 - \frac{m\alpha^2}{\pi\hbar^2}. \tag{9}$$

Only the first term is dependent on λ, so the minimum is obtained when this quadratic term vanishes. This determines the optimal value for λ, and thus the best estimate for the ground state energy is

$$E = -\frac{m\alpha^2}{\pi\hbar^2}. \tag{10}$$

For the trial function $f(x) = \mathrm{e}^{-\lambda|x|}$, a similar calculation yields

$$E[f] = \frac{\frac{\hbar^2}{2m}\lambda - \alpha}{1/\lambda} = \Big(\frac{\hbar\lambda}{\sqrt{2m}} - \frac{\sqrt{2m}\alpha}{2\hbar}\Big)^2 - \frac{m\alpha^2}{2\hbar^2}. \tag{11}$$

Again, we can choose λ so that the quadratic term vanishes. Since $-\frac{m\alpha^2}{2\hbar^2} < -\frac{m\alpha^2}{\pi\hbar^2}$, the estimate obtained using $f(x) = \mathrm{e}^{-\lambda|x|}$ is the best one.

Problem 3

To solve this problem, we must calculate the expectation value of the Hamiltonian for $z \geq 0$:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + Fz \tag{12}$$

using the trial function $f(z)$:

$$E[f] = \frac{\int_0^\infty f^* \hat{H} f dz}{\int_0^\infty |f|^2 dz}. \tag{13}$$

We will need three integrals which can be solved by standard techniques:

$$\begin{aligned} \int_0^\infty |f|^2 dz &= \alpha^{-3/2}\sqrt{\pi}/4, \\ -(\hbar^2/2m)\int_0^\infty f f'' dz &= (\hbar^2/2m)\frac{3}{8}\sqrt{\pi/\alpha}, \\ F\int_0^\infty z|f|^2 dz &= \frac{1}{2}F\alpha^{-2}. \end{aligned} \tag{14}$$

This gives us

$$E[f] = \frac{\hbar^2}{2m}\frac{3\alpha}{2} + \frac{2F}{\sqrt{\pi\alpha}}. \tag{15}$$

To find the minimum, we calculate the derivative with respect to α and set it to zero. This gives:

$$\alpha = \left(\frac{2}{3\sqrt{\pi}}F\frac{2m}{\hbar^2}\right)^{2/3}. \tag{16}$$

Substituting this back into $E[f]$, we find the minimum value

$$E = 3\left(\frac{3}{2\pi}\right)^{1/3}\left(\frac{\hbar^2}{2m}\right)^{1/3}F^{2/3}. \tag{17}$$