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Solutions FY2045 fall 2021

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Problem 1

a) After integration by parts, the expectation value of the kinetic energy is

$$\langle\psi|T|\psi\rangle = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}|\psi'(x)|^2\,dx\,. \tag{1}$$

The derivative of the trial wavefunction is

$$\psi'(x) = -\alpha^{\frac{3}{2}}\frac{|x|}{x}e^{-\alpha|x|}\,. \tag{2}$$

Integrating, we find

$$\begin{aligned}\langle\psi|T|\psi\rangle &= \frac{\hbar^2}{2m}\alpha^3\int_{-\infty}^{\infty}e^{-2\alpha|x|}\,dx\,.\\ &= \underline{\underline{\frac{\hbar^2}{2m}\alpha^2}}\,.\end{aligned} \tag{3}$$

Comment: One can also use the standard expression for T, but that requires finding $\psi''(x)$. Due to the factor $\frac{x}{|x|}$, this gives rise to a delta-function

$$\psi'' = -2\alpha^{\frac{3}{2}}\delta(x)e^{-\alpha|x|} + \alpha^{\frac{5}{2}}e^{-\alpha|x|} . \tag{4}$$

Using the expression for ψ and ψ'' in the expression

$$\langle\psi|T|\psi\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi(x)\psi''(x)\,dx , \tag{5}$$

yields the same result, Eq. (3).

b) The contribution to the energy from the potential term is

$$\begin{aligned}\langle\psi|V|\psi\rangle &= \int_{-\infty}^{\infty}\psi^*(x)V(x)\psi(x)\,dx = \frac{1}{2}m\omega^2\alpha\int_{-\infty}^{\infty}x^2e^{-2\alpha|x|}\,dx \\ &= \underline{\underline{\frac{1}{4}m\omega^2\frac{1}{\alpha^2}}} .\end{aligned} \tag{6}$$

c) The total energy is then

$$E(\alpha) = \underline{\underline{\frac{\hbar^2\alpha^2}{2m} + \frac{1}{4}m\omega^2\frac{1}{\alpha^2}}} . \tag{7}$$

The potential energy gets smaller as α gets larger. This corresponds to a wavefunction that is located near the origin (near the minimum of $V(x)$). On the other hand, the kinetic energy prefers a small value of α implying that the gradient be as small as possible. Thus there is a competition between these terms and the optimum is found by extremizing E as a function of α. $dE/d\alpha = 0$ yields

$$\frac{\hbar^2\alpha}{m} - \frac{1}{2}\frac{m\omega^2}{\alpha^3} = 0 , \tag{8}$$

or

$$\alpha^2 = \underline{\underline{\frac{1}{\sqrt{2}}\frac{m\omega}{\hbar}}} . \tag{9}$$

The corresponding energy is

$$E_{\rm opt} = \underline{\underline{\frac{1}{2}\sqrt{2}\hbar\omega}} , \tag{10}$$

which is higher than the exact ground-state energy by a factor of $\sqrt{2}$. This is not particular impressive. Finally, we note that the

$$\left.\frac{d^2E}{d\alpha^2}\right|_{\alpha^2=\frac{1}{\sqrt{2}}\frac{m\omega}{\hbar}} = \frac{4\hbar^2}{m} > 0 , \tag{11}$$

showing that the extremum in fact is a minimum.

Problem 2

a) Since $\mathcal{H}$ is nonempty there is a nonzero vector that we denote by $|\psi\rangle$. Either $b|\psi\rangle = 0$ or $b|\psi\rangle = |\chi\rangle \neq 0$. In the first case we are done, so we focus on the second case. We find

$$b|\chi\rangle \quad = \quad b^2|\psi\rangle = \underline{\underline{0}}\,, \tag{12}$$

where we in the second step have used that $\{b, b\} = 2b^2 = 0$. We denote by $|0\rangle$ the state annihilated by $\hat{b}$.

b) Assume $b^\dagger|0\rangle = 0$. Then $bb^\dagger|0\rangle = 0$ or $(1 - b^\dagger b)|0\rangle = |0\rangle = 0$, which is a contradiction. Consider $|1\rangle = \hat{b}^\dagger|0\rangle$, which yields $\langle 1| = \langle 0|\hat{b}$. Thus

$$\langle 1|1\rangle \quad = \quad \langle 0|bb^\dagger|0\rangle = \langle 0|1 - b^\dagger b|0\rangle = \langle 0|0\rangle = \underline{\underline{1}}\,, \tag{13}$$

where we have used the anticommutation relation $\left\{b, b^\dagger\right\} = 1$. Thus $|1\rangle$ is a normalized vector. Moreover, we find

$$b|1\rangle \quad = \quad bb^\dagger|0\rangle = (1 - b^\dagger b)|0\rangle = \underline{\underline{|0\rangle}}\,. \tag{14}$$

In the same way, we obtain

$$b^\dagger|1\rangle \quad = \quad b^\dagger b^\dagger|0\rangle = \underline{\underline{0}}\,. \tag{15}$$

c) The results above show that the space spanned by the vectors $|0\rangle$ and $|1\rangle$ is closed under the action of the operators 1, b and $b^\dagger$, and $bb^\dagger$ (or $b^\dagger b$). Any product of b and $b^\dagger$ can be reduced to these four using the anticommutation relations. It is therefore closed under the action of any product of these operators. Thus they span the space and since they are linearly independent, they form a basis. The space is therefore two-dimensional.

d) The operators b is not hermitian, which follows from the calculations above. Assume b is hermitian. Then $b|0\rangle = b^\dagger|0\rangle = |1\rangle$, but we also know that b annihilates the state $|0\rangle$, implying that $|1\rangle = 0$, which is a contradiction. The calculations above also show that the operator b has the matrix representation

$$b \quad = \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\,. \tag{16}$$

This confirms that $b \neq b^\dagger$. The eigenvector of this matrix is $|0\rangle$ with eigenvalues zero, i.e.

$$b|0\rangle \quad = \quad \underline{\underline{0|0\rangle}}\,. \tag{17}$$

In the same manner, we can calculate the eigenvectors of $b^\dagger$. One finds

$$b^\dagger|1\rangle \quad = \quad \underline{\underline{0|1\rangle}}\,. \tag{18}$$

Note that there is only one eigenvector in each case.

e) We must construct the 2×2 matrix representation of the Hamiltonian by calculating all its matrix elements. However, the above calculations suggest that $|0\rangle$ and $|1\rangle$ are eigenvectors of H. Explicit calculations show

$$H|0\rangle = \frac{1}{2}\hbar\omega(b^\dagger b - bb^\dagger)|0\rangle = \underline{\underline{-\frac{1}{2}\hbar\omega|0\rangle}} \,, \tag{19}$$

$$H|1\rangle = \frac{1}{2}\hbar\omega(b^\dagger b - bb^\dagger)|1\rangle = \underline{\underline{\frac{1}{2}\hbar\omega|1\rangle}} \,. \tag{20}$$

Thus the energy of the state $|0\rangle$ is $E_0 = \underline{\underline{-\frac{1}{2}\hbar\omega}}$ and the energy of the state $|1\rangle$ is $E_1 = \underline{\underline{\frac{1}{2}\hbar\omega}}$.

f) This follows automatically from $b^\dagger|1\rangle = b^\dagger b^\dagger|0\rangle = 0$, since by acting with $b^\dagger b^\dagger$ on the vacuum state $|0\rangle$, one tries to construct a state with two identical fermions in the same state. The number operator is

$$N = \underline{\underline{b^\dagger b}} \,, \tag{21}$$

since $b^\dagger b|0\rangle = 0|0\rangle$ and $b^\dagger b|1\rangle = |1\rangle$.

Problem 3

a) The expectation value of the first term in $H_{\rm hf}$ in a state $|\psi\rangle$ is proportional to

$$\left\langle \psi \left| \frac{[3(\mathbf{S}_p \cdot \mathbf{e}_r)(\mathbf{S}_e \cdot \mathbf{e}_r) - \mathbf{S}_p \cdot \mathbf{S}_e]}{r^3} \right| \psi \right\rangle \,. \tag{22}$$

For spherically symmetric states, i.e. s-states, the first term above can be replaced by

$$\frac{1}{4\pi}\frac{4\pi}{3}\frac{3\mathbf{S}_p \cdot \mathbf{S}_e}{r^3} = \frac{\mathbf{S}_p \cdot \mathbf{S}_e}{r^3} \,, \tag{23}$$

since multiplying the integrand by $|\psi^2|$ does not change the angular average. The result then follows.

b) In the absence of the spin-spin interaction, the energy eigenstates of hydrogen are also eigenstates of $\mathbf{S}_e^2$, $\mathbf{S}_p^2$, $S_{e,z}$, and $S_{p,z}$. The spin part of the eigenstates are denoted by $|S_{e,z}S_{p,z}\rangle$, where $S_{e,z}$ and $S_{p,z}$ are the z-component of spin of the electron and the proton, respectively. Since $\mathbf{S}^2 = \frac{3}{4}\hbar^2$ always, we suppress these quantum numbers for notational simplicity. The perturbation $\mathbf{S}_e \cdot \mathbf{S}_p$ does not commute with $S_{e,z}$ or $S_{p,z}$ but commutes with $\mathbf{S}^2$, and S_z, where $\mathbf{S} = \mathbf{S}_e + \mathbf{S}_p$. [1] The correct zeroth-order wavefunctions are then $|SS_z\rangle$, where S is the total spin quantum number and S_z is its z-component. Since the electron

[1] This is analogous to the case where we consider spin-orbit coupling.

and the proton both are spin-$\frac{1}{2}$ particles, the total spin is either $S = 0$ or $S = 1$. We next write

$$\boldsymbol{S}_e \cdot \boldsymbol{S}_p = \frac{1}{2}\left[S^2 - \hat{S}_e^2 - S_p^2\right] . \tag{24}$$

which implies that

$$\langle SS_z|\boldsymbol{S}_e \cdot \boldsymbol{S}_p|SS_z\rangle = \frac{1}{2}\hbar^2\left[S(S+1) - \frac{3}{2}\right] , \tag{25}$$

The first-order energy correction is then

$$E_{\rm hf}^{(1)} = \frac{\mu_0 g e^2}{3m_p m_e}\langle SS_z|\boldsymbol{S}_e \cdot \boldsymbol{S}_p|SS_z\rangle \, |\psi_{100}(0)|^2 , \tag{26}$$

where the last factor comes from integrating over space using the delta-function. This yields

$$E_{\rm hf}^{(1)} = \frac{g\hbar^4}{3m_p m_e^2 c^2 a^4}\begin{cases} \frac{1}{4} , & S = 1 , \\ -\frac{3}{4} , & S = 0 , \end{cases} , \tag{27}$$

where we have used that $\psi_{100}(0) = \frac{1}{\sqrt{\pi a^3}}$, $a = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ and $\mu_0\epsilon_0 = 1/c^2$.
Comment: Calculating the numerical value of the energy shift by plugging in numbers, one finds a frequency of 1420 Mhz or a wavelength of 21cm. This is shown in Fig. 1. This line which is in the microwave region of the electromagnetic spectrum, and it is observed frequently in radio astronomy. It is arguably the most important line in astronomy.

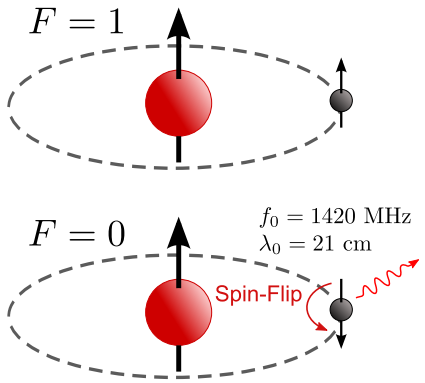

Figure 1: Hyperfine structure and 21 cm line in hydrogen.