

### A3 2009 Answers

1. Two-slit experiment for electrons: a source shoots electrons at a screen with two slots, beyond which is a photographic plate to detect the electrons. The plate shows an oscillatory pattern similar to the diffraction pattern of light traversing two slots.

Classically, one expects the plate to show the sum of two Gaussians,  $p(x) = p_1(x) + p_2(x)$ . With probability amplitudes, however, one gets an interference term:  $p(x) = |A_1(x) + A_2(x)|^2 = |A_1(x)|^2 + |A_2(x)|^2 + 2\text{Re}(A_1(x)A_2^*(x))$ . The last term is different from the classical prediction, and leads to the observed oscillatory pattern.

2. The total wavefunction must be antisymmetric under particle interchange.

If the two electrons have the same spatial wavefunctions, then the spin part must be antisymmetric. If the spin ket  $|m_1 m_2\rangle$  specifies the spins of the first and second electrons, then the total wavefunction must be

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{x}_1)\psi(\mathbf{x}_2)\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle].$$

The total spin is 0 (recall that the triplet spin state is symmetric and has  $S = 1$ ).

3. The state  $|\psi, t\rangle$  is

$$|\psi, t\rangle = ae^{-iE_1 t/\hbar}|E_1\rangle + be^{-iE_2 t/\hbar}|E_2\rangle$$

The probability of finding the system in state  $|E_1\rangle$  is  $|\langle E_1|\psi, t\rangle|^2 = a^2$ . For  $|E_2\rangle$ , it is  $|\langle E_2|\psi, t\rangle|^2 = b^2$ , and for the given superposition, it is

$$\left|\frac{1}{\sqrt{2}}(\langle E_1| + \langle E_2|)|\psi, t\rangle\right|^2 = \frac{1}{2}\left[a^2 + b^2 + 2ab\cos\frac{(E_1 - E_2)t}{\hbar}\right]$$

4. Recall that a commutator of operators must be thought of as working on an arbitrary state. But if we have a complete set of eigenstates  $|i\rangle$ , then any state can be written  $|\psi\rangle = \sum_i c_i|i\rangle$ .

$$\begin{aligned}[A, B]|\psi\rangle &= (AB - BA)\sum_i c_i|i\rangle \\ &= \sum_i a_i b_i c_i|i\rangle + \sum_i b_i a_i c_i|i\rangle \\ &= 0\end{aligned}$$

5. Adiabatic principle: if a system is initially in the  $k$  energy eigenstate, it will stay in this state under slow time evolution of the Hamiltonian.

The energy of the oscillator at  $t = t_1$  is  $E = 3\hbar\omega_0$ .

The reason is that the energy eigenstates of a harmonic oscillator with frequency  $\omega$  is  $E_n = \hbar\omega(n + \frac{1}{2})$ . At  $t = 0$ , the given energy indicates the oscillator is in state  $|1\rangle$ . At  $t = t_1$ , it remains in that state, and the energy is now  $E = \hbar 2\omega_0(1 + \frac{1}{2})$ .

6. The operators do not modify the time-dependent phase, so we can ignore them in this calculation (alternatively, compute one term and see them drop out). We have

$$\begin{aligned}\psi \frac{d\psi^*}{dx} &= -ik(|A|^2 - |B|^2 - AB^* e^{2ikx} + A^* B e^{-2ikx}) \\ J &= \frac{\hbar k}{m}(|A|^2 - |B|^2)\end{aligned}$$

Both terms are of the form velocity  $\times$  probability density, where  $v = \hbar k/m$  and the probability densities  $|A|^2$  and  $|B|^2$  correspond to the two parts of the wavefunction. The relative sign between the two terms reflect the fact that the  $A$  part is right-moving, and the  $B$  part is left-moving.

7. The Hamiltonian inside the box

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2$$

The wavefunction must vanish at the edges of the box, so it must take the form

$$\psi(\mathbf{x}) = A \sin \frac{\pi n_x x}{l_x} \sin \frac{\pi n_y y}{l_y} \sin \frac{\pi n_z z}{l_z}$$

Plugging this into the TISE,  $H\psi = E\psi$ , gives

$$E = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2} \right)$$

8. Since  $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ , and using the fact that each electron has spin 1/2 (and thus the eigenvalue of  $\mathbf{S}_i^2$  is  $s_i(s_i + 1) = 3/4$ ,

$$\begin{aligned}\mathbf{S}^2 &= \mathbf{S}_1^2 + \mathbf{S}_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \\ \mathbf{S}_1 \cdot \mathbf{S}_2 &= \frac{1}{2}(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2) \\ &= \frac{1}{2}(\mathbf{S}^2 - \frac{3}{2}) \\ H &= \frac{m}{2} \left( \mathbf{S}^2 - \frac{3}{2} \right) + \mu B S_z\end{aligned}$$

where the fact that  $\mathbf{B}$  is only the  $z$  direction has been used as well. In this form, it is clear that  $H$  commutes with  $\mathbf{S}^2$  and  $S_z$ , assuming, as given, that  $[\mathbf{S}^2, S_z] = 0$ .

The energy eigenvalues are as follows:

$$\begin{aligned}H|1, 1\rangle &= \left( \frac{m}{4} + \mu B \right) |1, 1\rangle \\ H|1, 0\rangle &= \frac{m}{4} |1, 0\rangle \\ H|1, -1\rangle &= \left( \frac{m}{4} - \mu B \right) |1, -1\rangle \\ H|0, 0\rangle &= -\frac{3m}{4} |0, 0\rangle\end{aligned}$$

Degeneracies appear for  $B = 0$  and  $B = \pm m/\mu$ .

9. Adding and subtracting  $a$  and  $a^\dagger$ , one obtains

$$\begin{aligned}x &= \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \\p &= -i\sqrt{\frac{m\hbar\omega}{2}}(a - a^\dagger)\end{aligned}$$

From these, we obtain

$$\begin{aligned}\bar{x} &= \langle n|x|n \rangle \propto \langle n|a + a^\dagger|n \rangle = 0 \\ \bar{p} &= \langle n|p|n \rangle \propto \langle n|a - a^\dagger|n \rangle = 0\end{aligned}$$

For the variances, we observe that  $\langle n|(a + a^\dagger)^2|n \rangle = \langle n|(aa^\dagger + a^\dagger a|n \rangle = \langle n|(2N + 1)|n \rangle = 1 + 2n$ , and similarly for  $(a - a^\dagger)$ .

$$\begin{aligned}\Delta_x^2 &= \frac{\hbar}{2m\omega}(2n + 1) \\ \Delta_p^2 &= \frac{m\hbar\omega}{2}(2n + 1) \\ \Delta_x\Delta_p &= \hbar\left(n + \frac{1}{2}\right) \geq \frac{\hbar}{2}\end{aligned}$$

thus verifying the uncertainty relationship for all  $n$ .

From first-order perturbation theory,

$$\delta E_n = \lambda \langle n|x^k|n \rangle \propto \langle n|(a + a^\dagger)^k|n \rangle$$

If  $k$  is odd, all the terms in  $(a + a^\dagger)^k$  have an odd number of operators, so there cannot be an equal number of creation and annihilation operators, so  $\delta E_n$  always vanishes.

For  $k = 4$ , we can square

$$(a + a^\dagger)^2 = (aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$$

keeping only those terms with an equal number of  $a$  and  $a^\dagger$ . This results in

$$\begin{aligned}\langle n|(a + a^\dagger)^4|n \rangle &= 6n^2 + 6n + 3 \\ \delta E_n &= \lambda \left(\frac{\hbar}{2m\omega}\right)^2 (6n^2 + 6n + 3)\end{aligned}$$

We know that  $\langle n|H|n \rangle = \hbar\omega(n + \frac{1}{2})$ . The consistency condition is therefore

$$\lambda \left(\frac{\hbar}{2m\omega}\right)^2 (6n^2 + 6n + 3) \ll \hbar\omega\left(n + \frac{1}{2}\right)$$

which puts an upper limit on  $n$ .

The variance  $\Delta_x$  increases with  $n$ , so the wavefunction is extending over larger  $x$  values. However, at larger  $x$  values, the perturbation becomes larger, until the approximation becomes invalid.

**10.** The radial part of the Hamiltonian (the  $r$  derivatives in one, and the  $p_r$  term in the other) can be verified independent of the rest.

For the angular part, we first see that  $\mathbf{L}^2 = L_+L_- + L_z^2 - L_z$ , using the commutation relation  $[L_x, L_y] = iL_z$ . One then works from both sides to match the two angular parts.

Inside the potential well, we use the fact that the  $Y_{lm}$  are eigenfunctions of the  $\mathbf{L}^2$  operator to isolate the radial part:

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} R = ER$$

For the  $l = 0$  case, it is straightforward to verify that the given wavefunction satisfies the equation. The energy is given by  $E = \hbar^2 k^2 / 2m$ . The wavefunction vanishes at  $r = a$ , which imposes the condition  $k = n\pi/a$ , so the energy levels are

$$E = \frac{\pi^2 \hbar^2 n^2}{2ma^2}$$

where  $n \geq 1$  is an integer.

For  $l = 1$ , the solution is given in the problem (you don't have to verify it). In this case, however, since  $R = (B/r^2)(kr \cos kr - \sin kr)$ , the boundary condition implies  $\tan ka = ka$ . For large values of  $ka$ , we have  $ka \approx \pi(n + \frac{1}{2})$ , with  $n$  an integer, in which case the energy spectrum for large  $n$  is

$$E \approx \frac{\pi^2 \hbar^2}{2ma^2} \left( n + \frac{1}{2} \right)^2$$

**11.** The TISE is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V_0(\delta(x+a) + \delta(x-a))\psi = E\psi$$

Integrating this equation over the small interval  $(x - \epsilon, x + \epsilon)$ , and then taking the limit as  $\epsilon \rightarrow 0$ , we see that the right-hand side of the equation vanishes since  $\psi$  is continuous at  $x = a$ . The left-hand side, however, becomes

$$-\frac{\hbar^2}{2m}(\psi'(a^+) - \psi'(a^-)) + V_0\psi(a) = 0$$

so the difference in  $\psi'$  is  $2mV_0\psi(a)/\hbar^2$ . A similar analysis holds for  $x = -a$ .

$H$  is invariant under the transformation  $x \rightarrow -x$ , so  $[H, P] = 0$ , where  $P$  is the parity operator. As a result, one can choose common eigenstates of  $H$  and  $P$ , and the eigenstates of  $P$  are either symmetric or antisymmetric in  $x$ .

The general form of the  $E < 0$  wavefunction is

$$\psi(x) = \begin{cases} Ae^{\kappa x} & x < -a \\ Be^{\kappa x} + Ce^{-\kappa x} & -a < x < a \\ De^{-\kappa x} & x > a \end{cases}$$

with  $\kappa^2 = 2m|E|/\hbar^2$ . For the symmetric solution, this becomes

$$\psi(x) = \begin{cases} Ae^{\kappa x} & x < -a \\ B \cosh(\kappa x) & -a < x < a \\ Ae^{-\kappa x} & x > a \end{cases}$$

The matching conditions at  $x = a$  are  $\psi(a^-) = \psi(a^+)$  and  $\psi'(a^+) - \psi'(a^-) = 2mV_0\psi(a)/\hbar^2$  yield

$$\begin{aligned} B \cosh(\kappa a) &= Ae^{-\kappa a} \\ -\kappa Ae^{-\kappa x} - B\kappa \sinh(\kappa a) &= 2mV_0Ae^{-\kappa a}/\hbar^2 \end{aligned}$$

which, eliminating  $B$ , leads to

$$\tanh \kappa a = \frac{\lambda}{\kappa a} - 1$$

where  $\lambda = -2mV_0a/\hbar^2$ .

The antisymmetric derivation follows similar lines, but with the wavefunction form

$$\psi(x) = \begin{cases} Ae^{\kappa x} & x < -a \\ B \sinh(\kappa x) & -a < x < a \\ -Ae^{-\kappa x} & x > a \end{cases}$$

The result is then

$$\tanh \kappa a = \left( \frac{\lambda}{\kappa a} - 1 \right)^{-1}$$

as required.

The number of solutions is obtained by counting the intersections on each side of the  $\kappa a$  equations. In the symmetric case, the tanh term increases monotonically from 0 to 1 as  $\kappa a \rightarrow \infty$ , while the right-hand side decreases monotonically from infinity to  $-1$ . There is therefore precisely one solution.

For the antisymmetric case, the right-hand side is 0 at  $x = 0$  and increases to  $\infty$  as  $x \rightarrow \lambda$ ; the function is also concave, while tanh is convex. The first derivative at  $x = 0$  can thus be used to decide whether the curves intersect. The result is that an antisymmetric bound state exists only for  $\lambda > 1$ .

**12.** The Hamiltonians  $H_0(\mathbf{r}_1)$  and  $H_0(\mathbf{r}_2)$  give the kinetic energies and Coulomb interactions of the two electrons, independently, with the nucleus. The last term represents the Coulomb interaction between the two electrons.

The radial derivatives on the given wavefunction give

$$\frac{1}{r_i^2} \frac{\partial}{\partial r_i} \left( r_i^2 \frac{\partial \psi}{\partial r_i} \right) = \frac{Z^2}{a_0^2} \psi - \frac{2Z}{a_0 r_i} \psi$$

which can be plugged into the ‘‘unperturbed’’ TISE,  $(H_0 + H_1)\psi = E\psi$ . The second part of the above expression cancels with the individual Coulomb interactions with the nucleus. The energy is then

$$E_0 = -\frac{4\hbar^2}{m_e a_0^2} = -\frac{4e^2}{4\pi\epsilon_0 a_0} = -8\mathcal{R}$$

where  $\mathcal{R}$  is the Rydberg constant.

The normalization integral is

$$\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 |\psi(\mathbf{r}_1, \mathbf{r}_2)|^2 = \frac{16Z^6}{a_0^6} \left( \int_0^\infty r^2 e^{-2Zr/a_0} dr \right)^2 = 1$$

In order to evaluate  $\langle \psi | H | \psi \rangle$ , it is easiest to look at the “unperturbed” Hamiltonian first:

$$\langle \psi | H_0 + H_1 | \psi \rangle = -\frac{\hbar^2 Z^2}{m_e a_0^2} + \frac{\hbar^2 (Z - 2)}{m_e a_0} \langle \psi | (r_1^{-1} + r_2^{-1}) | \psi \rangle$$

The individual integrals are

$$\begin{aligned} \langle \psi | r_i^{-1} | \psi \rangle &= \frac{Z^6}{\pi^2 a_0^6} \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 r_i^{-1} e^{-2Z(r_1+r_2)/a_0} \\ &= \frac{Z}{2a_0} \left( \int_0^\infty x e^{-x} dx \right) \left( \int_0^\infty y^2 e^{-y} dy \right) \\ &= \frac{Z}{a_0} \end{aligned}$$

which, combined, gives

$$\langle \psi | H_0 + H_1 | \psi \rangle = 2\mathcal{R}(Z^2 - 4Z)$$

The interaction term is

$$\begin{aligned} \langle \psi | H_I | \psi \rangle &= \frac{e^2 Z^6}{4\pi\epsilon_0 \pi^2 a_0^6} \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 e^{2Z(r_1+r_2)/a_0} / |\mathbf{r}_1 - \mathbf{r}_2| \\ &= \frac{e^2 Z^6}{4\pi\epsilon_0 \pi^2 a_0^6} \frac{a_0^5}{32Z^5} 20\pi^2 \\ &= \frac{5}{4} \mathcal{R} Z \end{aligned}$$

using the hint given in the problem. The combination is then

$$\langle \psi | H | \psi \rangle = 2\mathcal{R} \left( Z^2 - \frac{27}{8} Z \right)$$

which, when minimized, gives  $Z_{min} = 27/16$  and energy  $-8\mathcal{R}(27/32)^2$ .

The result that  $Z_{min} < 2$  reflects the fact that part of the nucleus charge seen by the electron is partially “screened” by the other electron. We have also found that  $E(Z_{min}) > E_0$ , so the atom is less strongly bound when the electron interaction is taken into account, explained equivalently by the mutual repulsion of the electrons or the screening.