4141 HW 4

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1a

The stationary states of an electron in an infinite square well of width a are

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

The energy is related to the wavenumber of the above functions by $k = \frac{\sqrt{2mE_n}}{\hbar} \Leftrightarrow E_n = \frac{k^2\hbar^2}{2m}$ using the definition of k from the time-independent Schrödinger equation. Therefore,

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

$$\Rightarrow E_1 = \frac{\pi^2\hbar^2}{2ma^2} = \frac{\pi^2(1.05 \times 10^{-34}\,\mathrm{J\cdot s})^2}{2(9.11 \times 10^{-31}\,\mathrm{kg})(10^{-10}\,\mathrm{m})^2} = 6.05 \times 10^{-19}\,\mathrm{J}$$

$$E_2 = \frac{2\pi^2\hbar^2}{ma^2} = 4E_1 = 2.42 \times 10^{-18}\,\mathrm{J}$$

$$E_3 = \frac{9\pi^2\hbar^2}{2ma^2} = 9E_1 = 5.45 \times 10^{-18}\,\mathrm{J}$$

1b

The energy difference between the ground and second excited states are

$$E_3 - E_1 = 4.84 \times 10^{-18}\,\mathrm{J}$$

This corresponds to a photon frequency of

$$f = \frac{E}{h} = \frac{4.84 \times 10^{-18}\,\mathrm{J}}{6.67 \times 10^{-34}\,\mathrm{J\cdot s}} = 7.26 \times 10^{15}\,\mathrm{Hz}$$

needed to excite the electron. As the electron de-excites, it will enter the first excited state, and then the ground state from there. The corresponding energies are

$$E_{32} = E_3 - E_2 = 3.03 \times 10^{-18}\,\mathrm{J}$$

and

$$E_{21} = E_2 - E_1 = 1.82 \times 10^{-18}\,\text{J}$$

which correspond to photon frequencies

$$f_{32} = \frac{E_{32}}{h} = 4.54 \times 10^{15}\,\text{Hz}$$

$$f_{21} = \frac{E_{21}}{h} = 2.73 \times 10^{15}\,\text{Hz}$$

2

The time-dependent wave function is

$$\Psi(x,t) = Ae^{ikx - i\hbar k^2/2m} + Be^{-ikx - i\hbar k^2/2m}$$

The flux is defined as

$$J = \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right) =$$

$$\frac{i\hbar}{2m}\Bigg(\left[Ae^{ikx-i\hbar k^2/2m} + Be^{-ikx-i\hbar k^2/2m}\right]\cdot\left[-ikAe^{-ikx+i\hbar k^2/2m} + ikBe^{ikx+i\hbar k^2/2m}\right]$$

$$-\left[Ae^{-ikx+i\hbar k^2/2m} + Be^{ikx+i\hbar k^2/2m}\right]\cdot\left[ikAe^{ikx-i\hbar k^2/2m} - ikBe^{-ikx-i\hbar k^2/2m}\right]\Bigg)$$

$$= \frac{i\hbar}{2m}\left(2ik(B^2 - A^2)\right) = \frac{k\hbar}{2m}(B^2 - A^2)$$

3

If ψ is real, the expectation value of $x\frac{dV}{dx}$ is

$$\int_{-\infty}^{\infty}\psi(x)x\frac{\partial V}{\partial x}\psi(x)dx = x\psi^2V\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}(2x\psi\psi' + \psi^2)V\,dx$$

Since the wave function must be normalized, it must limit to zero at both infinities, so the first term is zero. Noting that by definiton

$$\langle V\rangle = \int_{-\infty}^{\infty}\psi V\psi dx$$

this is therefore

$$= -\langle V\rangle - 2\int_{-\infty}^{\infty}\frac{\partial\psi}{\partial x}xV\psi dx$$

By the energy eigenvalue equation, this is

$$= -\langle V\rangle + \left(E + \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{\partial\psi}{\partial x}\right)^2 dx\right)$$

Since $E = T + V$, we may we may rewrite this as

$$= \langle T \rangle + \frac{\hbar^2}{2m} \left(\psi \frac{\partial \psi}{\partial x} \bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi \frac{\partial^2 \psi}{\partial x} dx \right) = \langle T \rangle + \langle T \rangle$$

Applying the Ehrenfest theorem achieves the desired result:

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{2} \left\langle x \frac{\partial V}{\partial x} \right\rangle$$

Since we use the Ehrenfest theorem anyway, it's no less valid a proof to simply note that the virial theorem holds in classical mechanics, so it must hold for expectation values in quantum mechanics.

4

Differentiating the eigenvalue equation

$$F(x) - \lim_{x' \to -\infty} F(x') = \lambda \psi(x)$$

where F is the antiderivative of $x\psi(x)$,

$$x\psi = \lambda \frac{\partial \psi}{\partial x}$$

By separation of variables,

$$\psi(x) = ce^{x^2/2\lambda}$$

Therefore, all nonzero real nubmers are eigenvalues of this operator. Since going from the integral to the the differential equation is only a forward implication and not an equivalence, we know all eigenvalues of the differential equation are eigenvalues of the integral equation but not the converse; we must therefore check if zero is an eigenvalue of the original operator. If it were, there would be a nonzero function such that for all x

$$\int_{-\infty}^{x} xf(x)dx = 0$$

which is clearly false. The square of ψ is

$$c^2 e^{x^2/\lambda}$$

If λ is negative, the integral of this square is

$$c^2 e^{1/|\lambda|} \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} c^2 e^{1/|\lambda|}$$

which exists; if λ is positive, the integrand would be proportional to e^{x^2} which diverges and so isn't integrable.

5a

Representing the sine as an exponential,

$$\psi(x,0) = N\left(\frac{e^{i\pi x/a} - e^{-i\pi x/a}}{2i}\right)^5$$

The total probability is then

$$1 = \int_{-\infty}^{\infty} N^2 \left(\frac{e^{i\pi x/a} - e^{-i\pi x/a}}{2i}\right)^{10} dx$$

Applying the binomial theorem,

$$= -\frac{N^2}{1024}\int_0^a \sum_{k=0}^{10}(-1)^k \binom{10}{k} e^{(10-k)i\pi x/a} e^{-ki\pi x/a} dx$$

$$= -\frac{N^2}{1024}\sum_{k=0}^{10}(-1)^k \binom{10}{k}\int_0^a e^{(10-2k)i\pi x/a}dx = -\frac{N^2}{1024}\sum_{k=0}^{10}(-1)^k\binom{10}{k}\left(\frac{a}{(10-2k)i\pi}e^{(10-2k)i\pi x/a}\bigg|_0^a\right)$$

This is zero for all k but 5, in which case we must return to the pentultimate expression and note that the integrand becomes one, so this becomes

$$= \frac{N^2}{1024}\binom{10}{5}a = aN^2\frac{252}{1024} = \frac{63}{256}aN^2$$

implying

$$N = \frac{16}{3\sqrt{7a}}$$

5b

The stationary states of the infinite square well are

$$\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) = \sqrt{\frac{2}{a}}\left(\frac{e^{in\pi x/a} - e^{-in\pi x/a}}{2i}\right)$$

The initial wave function, expressed using the binomial theorem once again, is

$$\psi(x,0) = \frac{N}{32i}\sum_{k=0}^{5}(-1)^k\binom{5}{k}e^{(5-2k)i\pi x/a}$$

Applying Fourier's trick to obtain the initial wave function as a linear combination of stationary states,

$$c_n = \int_{-\infty}^{\infty}\psi_n^*(x)\psi(x,0)dx = -\frac{N}{64}\sqrt{\frac{2}{a}}\sum_{k=0}^{5}(-1)^k\binom{5}{k}\int_0^a e^{i\pi(5-2k+n)x/a} - e^{i\pi(5-2k-n)x/a}dx$$

$$= -\frac{N}{64}\sqrt{\frac{2}{a}}\sum_{k=0}^{5}(-1)^k\binom{5}{k}\left(\frac{a}{i\pi(5-2k+n)}e^{i\pi(5-2k+n)x/a}\bigg|_0^a - \frac{a}{i\pi(5-2k-n)}e^{i\pi(5-2k-n)x/a}\bigg|_0^a\right)$$

The exponents are both integer multiples of $i\pi$ when evaluated at a and zero when evaluated at zero. When n is even, both exponents are odd multiples of $i\pi$, and vice versa. Therefore, the only n that survive are the even ones, and the antiderivative evaluations both evaluate to $e^{i(2j+1)\pi} - 1 = -2$. This then becomes

$$= \frac{N\sqrt{2a}}{32\pi i}\sum_{k=0}^{5}(-1)^k\binom{5}{k}\left(\frac{1}{(5-2k+n)} - \frac{1}{(5-2k-n)}\right)$$

This is equal to zero for all n where it is defined for every k, as can be seen by writing out two terms of the sum where $\binom{5}{k}$ would give the same number and noticing that rightmost factor is the same, but the signs are opposite. However, this is not a justified manpulation when $5 = 2k - n$ or $5 = 2k + n$; equivalently, whenever $n = 2k - 5$ or $n = 5 - 2k$. To determine the value when this happens, we need only go back to the original integral.

Since $k = 0, 1, 2, 3, 4, 5$ and $n \geq 1$, the only (n, k) pairs for which this happens are $(1, 3)$, $(3, 4)$, and $(5, 5)$ for the first term being one and $(5, 0)$, $(3, 1)$, and $(1, 2)$ for the second term being one. Notice that the other exponential and all terms from other values of k always integrate to zero since the n are all odd. The nonzero coefficients in the expansion are therefore

$$c_1 = -\frac{N}{64}\sqrt{\frac{2}{a}}\left((-1)^3\binom{5}{3}a - (-1)^2\binom{5}{2}a\right) = 20\frac{N\sqrt{2a}}{64}$$

$$c_3 = -\frac{N}{64}\sqrt{\frac{2}{a}}\left((-1)^4\binom{5}{4}a - (-1)^1\binom{5}{1}a\right) = -10\frac{N\sqrt{2a}}{64}$$

$$c_5 = -\frac{N}{64}\sqrt{\frac{2}{a}}\left((-1)^5\binom{5}{5}a - (-1)^0\binom{5}{0}a\right) = 2\frac{N\sqrt{2a}}{64}$$

These are properly normalized, so likely correct. The time evolution of the state is then the expansion in terms of stationary states with each term multiplied by $e^{-iE_n t/\hbar}$, i.e.

$$\Psi(x,t) = \frac{\sqrt{2/7}}{12}\left(20e^{-iE_1 t/\hbar} - 10e^{-iE_2 t/\hbar} + 2e^{-iE_3 t/\hbar}\right)$$

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

5c

The probability a particle is in energy state E_3 is the modulus-squared of the coefficient c_3:

$$P = |c_3|^2 = \left|-10\frac{\sqrt{2/7}}{12}\right|^2 = .1984$$