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FY2045 Solutions Problem set 1 fall 2023

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Problem 1

a) The ground-state wavefunction is

$$\psi_0(x) \quad = \quad \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\xi^2} \,. \tag{1}$$

This yields

$$\langle x^2\rangle \quad = \quad \sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty} dx\ x^2 e^{-\xi^2} = \sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty} dx\ x^2 e^{-m\omega x^2/\hbar} = \frac{\hbar}{\sqrt{\pi}m\omega}\int_{-\infty}^{\infty} dy\ y^2 e^{-y^2},$$

where in the last equality we have changed to the integration variable $y = \sqrt{m\omega/\hbar}x$. This integral can be looked up in a table, or solved in the following (rather lengthy) way: We insert a dummy variable a in the exponential, which we will set to 1 at the end of the calculation:

$$I_1(a) \equiv \int_{-\infty}^{\infty} dy\ y^2 e^{-ay^2} = -\frac{\partial}{\partial a}\int_{-\infty}^{\infty} dy\ e^{-ay^2} \equiv -\frac{\partial}{\partial a} I_0(a), \tag{2}$$

where we have defined

$$I_0(a) = \int_{-\infty}^{\infty} dy\ e^{-ay^2}. \tag{3}$$

This doesn't seem to help us much, but we can now use a trick. We will square this integral, calling the integration variables of one of the integrals x[1] and y:

$$(I_0(a))^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \; e^{-a(x^2+y^2)}. \tag{4}$$

We now switch to radial coordinates $r = \sqrt{x^2+y^2}$, for which the integration changes according to

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \; f(x,y) = \int_0^{2\pi} d\theta \int_0^{\infty} dr \; r \cdot f(r,\theta). \tag{5}$$

Applying this to the above integral, we get

$$(I_0(a))^2 = \int_0^{2\pi} d\theta \int_0^{\infty} dr \; re^{-ar^2} = 2\pi \int_0^{\infty} dr \; re^{-ar^2} = -\frac{\pi}{a} e^{-ar^2}\Big|_0^{\infty} = \frac{\pi}{a}. \tag{6}$$

Hence $I_0(a) = \sqrt{\pi/a}$, and[2]

$$I_1(a) = \frac{\sqrt{\pi}}{2a^{3/2}}. \tag{7}$$

Setting $a = 1$, we therefore get

$$\langle x^2 \rangle \;=\; \frac{\hbar}{\sqrt{\pi} m\omega} \cdot \frac{\sqrt{\pi}}{2} = \underline{\underline{\frac{\hbar}{2m\omega}}} \;. \tag{8}$$

This implies $\langle V \rangle = \langle \frac{1}{2} m\omega^2 x^2 \rangle = \frac{1}{4}\hbar\omega$. Since we know that the system is in the ground state, which is an energy eigenstate, we have $E = \langle E \rangle = \frac{1}{2}\hbar\omega$. Moreover, since $E = T + V$ we have $\langle E \rangle = \langle T \rangle + \langle V \rangle$, resulting in $\langle T \rangle = \frac{1}{4}\hbar\omega$. This yields

$$\langle p^2 \rangle \;=\; 2m\langle T \rangle = \underline{\underline{\frac{m\hbar\omega}{2}}} \tag{9}$$

We can of course obtain Eq. (9) directly by evaluating the integral

$$\langle p^2 \rangle \;=\; \int_{-\infty}^{\infty} |\hat{p}\psi_0|^2 \; dx \;.$$

b) Choosing $\hat{A} = \hat{x}\hat{p}$, and using the commutation relation identity $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$, yields

$$\begin{aligned} [\hat{p}^2, \hat{x}\hat{p}] &= [\hat{p}^2, \hat{x}]\hat{p} + \hat{x}[\hat{p}^2, \hat{p}] \\ &= \hat{p}[\hat{p}, \hat{x}]\hat{p} + [\hat{p}, \hat{x}]\hat{p}^2 = -2i\hbar\hat{p}^2 \qquad (10) \\ [\hat{x}^2, \hat{x}\hat{p}] &= [\hat{x}^2, \hat{x}]\hat{p} + \hat{x}[\hat{x}^2, \hat{p}] \\ &= \hat{x}^2[\hat{x}, \hat{p}] + \hat{x}[\hat{x}, \hat{p}]\hat{x} = 2i\hbar\hat{x^2} \;, \qquad (11) \end{aligned}$$

[1] Not to be confused with the position x used above

[2] Note that we could generate the solutions of the integrals $I_n = \int_{-\infty}^{\infty} dy \; y^{2n} e^{-ay^2}$ in the same way.

where for both cases we have used that the commutator of the of an operator with itself is zero. This gives

$$\frac{i}{\hbar}[\hat{H}, \hat{x}\hat{p}] = \frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \hat{x}\hat{p}\right] = \frac{\hat{p}^2}{m} - m\omega^2\hat{x}^2 = 2(\hat{T} - \hat{V}) \; . \tag{12}$$

Since $\hat{x}\hat{p}$ has no explicit time dependence, $\partial\hat{x}/\partial t = \partial\hat{p}/\partial t = 0$, we obtain

$$\frac{d}{dt}\langle xp \rangle = \underline{\underline{2(\langle T \rangle - \langle V \rangle)}} \; . \tag{13}$$

c) Since the right-hand side vanishes in a stationary state, we obtain

$$\langle T \rangle - \langle V \rangle = 0 \; . \tag{14}$$

This is in agreement with ***a***), where $\langle T \rangle = \frac{1}{2m}\langle p^2 \rangle = \langle V \rangle = \frac{1}{2}m\omega^2\langle x^2 \rangle = \frac{1}{4}\hbar\omega$.

Problem 2

a) The normalization integral is

$$\begin{aligned} 1 &= |A|^2 \int_{-\infty}^{\infty} [\psi_0^*(x) + \psi_1^*(x)][\psi_0(x) + \psi_1(x)]\, dx \\ &= |A|^2 \int_{-\infty}^{\infty} \left[|\psi_0(x)|^2 + |\psi_1(x)|^2\right]\, dx \\ &= 2|A|^2 \; , \end{aligned} \tag{15}$$

where we in the second line have used that the eigenfunctions are orthogonal and in the last line that they are normalized. This yields

$$A = \underline{\underline{\frac{1}{\sqrt{2}}}} \; , \tag{16}$$

where we have chosen the phase $\alpha = 0$, i.e. that A is real.

b) The wavefunction can be expanded in terms of the energy eigenfunctions as

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}} \; , \tag{17}$$

where c_n are expansion coefficients. For $t = 0$ we can read off the expansion coefficients from $\Psi(x,0)$ and find $c_0 = c_1 = \frac{1}{\sqrt{2}}$ and $c_n = 0$ for $n = 2, 3, 4....$ This yields

$$\Psi(x,t) = \underline{\underline{\frac{1}{\sqrt{2}}\left[\psi_0(x)e^{-\frac{i\omega}{2}t} + \psi_1(x)e^{-\frac{3i\omega}{2}t}\right]}} \; , \tag{18}$$

where we have used $E_n = \hbar\omega(\frac{1}{2} + n)$. In the same way we find

$$|\Psi(x,t)|^2 = \frac{1}{2}\left\{|\psi_0(x)|^2 + |\psi_1(x)|^2 + \psi_0(x)\psi_1(x)\left[e^{-i\omega t} + e^{i\omega t}\right]\right\}$$
$$= \underline{\underline{\frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\left[1 + 2\xi^2 + 2\sqrt{2}\xi\cos\omega t\right]e^{-\xi^2}}} . \tag{19}$$

where we have used that the basis functions $\psi_0(x)$ and $\psi_1(x)$ are real, and that the difference $E_1 - E_0 = \hbar\omega$.

c) The expectation value can be written as

$$\langle x \rangle = \int_{-\infty}^{\infty} dx\ \Psi(x,t)^* \hat{x} \Psi(x,t) = \int_{-\infty}^{\infty} dx\ x|\Psi(x,t)|^2 , \tag{20}$$

where have used $\hat{x} = x$, which we are free to move around since it is just a number. The time-independent terms in the integrand of Eq. (20) are odd (see Eq. (19), and remember that $\xi \propto x$) and so they vanish upon integration. The time-dependent term is even and yields

$$\langle x \rangle = \sqrt{\frac{2\hbar}{\pi m\omega}}\cos\omega t\int_{-\infty}^{\infty} d\xi\ \xi^2 e^{-\xi^2} = \underline{\underline{\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t}} , \tag{21}$$

where we first have rewritten the integral in terms of $\xi = \sqrt{m\omega/\hbar}x$, and then used the result for the integral from Problem 1, see Eq. (7).

Ehrenfest's theorem states that

$$m\frac{d}{dt}\langle x \rangle = \langle p \rangle, \quad \text{and} \quad \frac{d}{dt}\langle p \rangle = \langle -\nabla V \rangle , \tag{22}$$

where V is the potential energy of the system. Hence there are two ways to calculate $\langle p \rangle$ from Ehrenfest's theorem. Using the first equation, we get

$$\langle p \rangle = m\frac{d}{dt}\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t = \underline{\underline{-\sqrt{\frac{\hbar m\omega}{2}}\sin\omega t.}} \tag{23}$$

Using the second equation, we use the potential function for the oscillator, $V(x) = \frac{1}{2}m\omega^2 x^2$, such that $\nabla V = m\omega^2 x$ and therefore

$$\frac{d}{dt}\langle p \rangle = -m\omega^2\langle x \rangle .$$

Integration yields

$$\langle p \rangle = \underline{\underline{-\sqrt{\frac{m\omega\hbar}{2}}\sin\omega t}} . \tag{24}$$

The expectation value $\langle p \rangle$ can of course be calculated directly evaluating the integral

$$\langle p \rangle = \int_{-\infty}^{\infty} dx \; \Psi^*(x,t)\hat{p}\Psi(x,t) = \int_{-\infty}^{\infty} dx \; \Psi^*(x,t) \left[-i\hbar \frac{d}{dx} \right] \frac{1}{\sqrt{2}} \left[\psi_0(x) e^{-\frac{i\omega}{2}t} + \psi_1(x) e^{-\frac{3i\omega}{2}t} \right]. \tag{25}$$

We calculate the derivatives,

$$\frac{d}{dx}\psi_0 = -\sqrt{\frac{m\omega}{\hbar}}\xi\psi_0, \tag{26}$$

$$\frac{d}{dx}\psi_1 = \sqrt{\frac{2m\omega}{\hbar}} \left[1 - \xi^2 \right] \psi_0, \tag{27}$$

and insert them into the above equations, resulting in

$$\begin{aligned} \langle p \rangle = \frac{i}{2}\sqrt{m\omega\hbar} \int_{-\infty}^{\infty} dx \; & [\psi_0(x) e^{+i\omega t/2} + \sqrt{2}\xi\psi_0(x) e^{+3i\omega t/2}] \\ & \times [\xi\psi_0 e^{-i\omega t/2} + \sqrt{2}(\xi^2 + 1)\psi_0 e^{-i3\omega t/2}], \end{aligned} \tag{28}$$

where we have expressed the results in terms of ψ_0 for simplicity, and used the fact $\psi_n(x)$ are real functions. $|\psi_0|^2$ is an even function in ξ x, and all odd terms therefore disappear when performing the integral. This leaves the following terms,

$$\begin{aligned} \langle p \rangle &= i\sqrt{\frac{m\omega\hbar}{2}} \int_{-\infty}^{\infty} dx \; \left[\frac{m\omega}{\hbar} x^2 (e^{i\omega t} + e^{-i\omega t}) - e^{-i\omega t} \right] |\psi_0|^2 \\ &= i\sqrt{\frac{m\omega\hbar}{2}} \left[\frac{m\omega}{\hbar} \langle x^2 \rangle (e^{i\omega t} + e^{-i\omega t}) - e^{-i\omega t} \right], \end{aligned} \tag{29}$$

where we have inserted for ξ, and we have used the definition of the expectation value of x^2 in the ground state, and the normalization of ψ_0. Inserting the result $\langle x^2 \rangle = \hbar/(2m\omega)$ calculated in Problem 1a), we get

$$\langle p \rangle = i\sqrt{\frac{m\omega\hbar}{2}} \frac{e^{i\omega t} - e^{-i\omega t}}{2} = \underline{\underline{-\sqrt{\frac{\hbar m\omega}{2}}}} \sin\omega t, \tag{30}$$

which is in agreement with the result obtained using Ehrenfest's theorem.

Problem 3

a) Since the energy E must be real, k must be either purely real or purely imaginary. Imaginary k corresponds to plane waves, which extend over the entire range of x, and are therefore not bound states. The wavefunction of a bound state also must be normalizable to 1, which is not the case for plane waves (they are delta-function normalizable). Thus k must be real, corresponding to a negative energy, $E < 0$.

We could also argue more directly: Since the potential is zero at $x = \pm\infty$, we know that the energy of a bound state must be negative (and real) — otherwise it could in principle tunnel out of the well and escape to infinity. Hence, k must be real.

For $x > 0$ and $k > 0$, we must have $B = 0$ for ψ to be normalizable to one. For $x < 0$ and $k > 0$, $A = 0$ for the same reason, and the wavefunction can be compactly written as[3]

$$\psi(x) \quad = \quad \underline{\underline{Ae^{-k|x|}}} \, , \qquad\qquad k > 0 \, . \tag{31}$$

b) The normalization integral is

$$|A|^2 \int_{-\infty}^{\infty} e^{-2k|x|} \, dx \quad = \quad \frac{|A|^2}{k} \, . \tag{32}$$

This yields

$$A \quad = \quad \underline{\underline{\sqrt{k}}} \, , \tag{33}$$

where we have chosen A to be real, i.e. set the arbitrary phase $\alpha = 0$.

The Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m} \psi''(x) + \beta\delta(x)\psi(x) \right] \quad = \quad E\psi(x) \, . \tag{34}$$

Integrating this equation from $-\epsilon$ to ϵ, we get

$$\int_{-\epsilon}^{\epsilon} dx \, \left[-\frac{\hbar^2}{2m} \psi''(x) + \beta\delta(x)\psi(x) \right] = -\frac{\hbar^2}{2m} [\psi'(\epsilon) - \psi'(-\epsilon)] + \beta\psi(0) = E \int_{-\epsilon}^{\epsilon} dx \, \psi(x). \tag{35}$$

Taking the limit $\epsilon \to 0$ the right hand side disappears, and we are left with

$$\frac{\hbar^2}{2m} \left[\psi'(0^-) - \psi'(0^+) \right] + \beta\psi(0) \quad = \quad 0 \, . \tag{36}$$

The derivative of the wavefunction is

$$\psi'(x) \quad = \quad -k^{\frac{3}{2}} \frac{x}{|x|} e^{-k|x|} \, , \tag{37}$$

which yields

$$-\frac{\hbar^2}{2m} \left[-k^{\frac{3}{2}} - k^{\frac{3}{2}} \right] + \sqrt{k}\beta \quad = \quad 0 \, , \tag{38}$$

or

$$\beta \quad = \quad \underline{\underline{-\frac{\hbar^2 k}{m}}} \, . \tag{39}$$

We note that $\beta < 0$ in order to have a bound state. The binding energy is $E_B = -E = \frac{\hbar^2 k^2}{2m} = \frac{m\beta^2}{2\hbar^2}$.

[3] For $k < 0$ a similar argument applies and the wavefunction is $\psi(x) = e^{k|x|}$.