Part IB Physics : Lent 2020

QUANTUM PHYSICS EXAMPLES II
MODEL ANSWERS

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1. Quantum mechanically, let us define region 1 ($0 < x < a$) and region 2 ($a < x < 2a$). The wave function has wave vectors $k_1 = \sqrt{2mE/\hbar^2} = 5\pi/(2a)$ and $k_2 = \sqrt{2m(E - V_0)/\hbar^2} = 3\pi/(2a)$, respectively. Requiring that the boundary conditions at $x = 0$ and $x = 2a$ are satisfied ($\psi(0) = \psi(2a) = 0$), we obtain: $\psi_1(x) = A\sin(k_1 x)$ and $\psi_2(x) = B\sin[k_2(2a - x)] = B\sin(k_2 x)$. We must finally impose the boundary conditions at $x = a$:

$$A\sin(5\pi/2) = B\sin(3\pi/2)$$
$$Ak_1\cos(5\pi/2) = -Bk_2\cos(3\pi/2)\,.$$

The latter is automatically satisfied ($\cos(5\pi/2) = \cos(3\pi/2) = 0$) whereas the former requires $A = -B$ ($\sin(5\pi/2) = -\sin(3\pi/2) = 1$). Since

$$\int_0^a \sin^2(k_1 x)\,dx = \int_a^{2a} \sin^2(k_2 x)]\,dx = a/2\,, \qquad (*)$$

the correct normalisation choice is $A = 1/\sqrt{a}$ and

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{a}}\sin(k_1 x) & 0 < x < a \\ -\frac{1}{\sqrt{a}}\sin(k_2 x) & a < x < 2a \end{cases}$$

$$P_{\text{quantum}} = \frac{1}{a}\int_0^a \sin^2(k_1 x)\,dx = \frac{1}{2}$$

(which could have actually been argued directly from ($*$) without further calculations).

Classically, the probability $P_{\text{classical}}$ of finding the particle in region 1 ($0 < x < a$) is given by the ratio of the time t_1 spent in region 1 divided by the total time ($t_1 + t_2$, where t_2 is the time spent in region 2). The time spent in a region is given by the size of the region divided by the velocity of the particle in that region, $t_{1,2} = a/v_{1,2}$. And the velocity can be obtained from the kinetic energy, $v_{1,2} = \sqrt{2mE_{1,2}}$. Recalling that $E_1 = E \propto 25/8$ and $e_2 = E - V_0 \propto 9/8$, and noticing that all dimensional factors cancel out, after a few lines of algebra we obtain

$$P_{\text{classical}} = \frac{t_1}{t_1 + t_2} = \frac{v_2}{v_1 + v_2} = \frac{\sqrt{E - V_0}}{\sqrt{E} = \sqrt{E - V_0}} = \frac{3/(2\sqrt{2})}{5/(2\sqrt{2}) + 3/(2\sqrt{2})} = \frac{3}{8}\,.$$

2. A one-dimensional rectangular potential well of depth V_0 has width $2a$. Show that there is one and only one bound state for a particle of mass m if

$$\frac{2ma^2V_0}{\hbar^2} < \frac{\pi^2}{4}$$

Let us divide space into regions 1 ($x < -a$), 2 ($-a < x < a$), and 3 ($x > a$). A bound state exists if at least one of the energy eigenstates is negative, $E < 0$. The corresponding behaviour of the wavefunction is

$$\psi(x) = \begin{cases} A_1 \exp(\kappa x) & \text{region 1} \\ A_2 \cos(kx) & \text{region 2} \\ A_1 \exp(-\kappa x) & \text{region 1}\,, \end{cases} \qquad (**)$$

where $\kappa = \sqrt{-2mE/\hbar^2}$ and $k = \sqrt{2m(E + V_0)/\hbar^2}$ and we made use of two key observations: (i) the problem is symmetric in $x \leftrightarrow -x$, and therefore $|\psi(x)|^2 = |\psi(-x)|^2$ (in particular, this means that the term in region 2 must be proportional to either a $\sin(kx)$ or $\cos(kx)$, but not a linear combination thereof; also, $|A_3|^2 = |A_1|^2$); and (ii) the lowest energy state ought to be nodeless (which means we can focus only on the $\cos(kx)$ solution in region 2; and thence $A_3 = A_1$).
We then need to impose the correct boundary conditions (which are now identical at $x = -a$ and $x = a$):

$$A_1 \exp(-\kappa a) = A_2 \cos(ka)$$
$$A_1 \kappa \exp(-\kappa a) = A_2 k \sin(ka)\,.$$

Taking the ratio of the two equations, $\kappa = k \tan(ka)$, and expressing it in terms of the dimensionless variable $x = E/V_0 \in (-1, 0)$, we obtain

$$\sqrt{\frac{-x}{1+x}} = \tan\left[\sqrt{\frac{2ma^2V_0}{\hbar^2}}\sqrt{1+x}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\sqrt{1+x}\right]\,.$$

The l.h.s. diverges for $x \to -1$ and decreases monotonically down to 0 at $x = 0$. The r.h.s. vanishes at $x = -1$ and increases monotonically up to the well-known singular discontinuity when the argument equals $\pi/2$. Therefore a solution (intersection point) always exists.
It is unique if the first excited state is unbound. In order to check this, we ought to replace cos with sin in Eq. ($**$), as we expect the first excited state to be odd rather than even. One could repeat the procedure above to derive the desired result. Alternatively, one can observe that the continuity of the derivative of the wave function at the boundary requires the sinusoidal function to be increasing / decreasing at $x = -a$ / $+a$, respectively, and therefore $ka > \pi/2$. The energy of the first excited state is therefore bounded from below by

$$\frac{\hbar^2\pi^2}{8ma^2} - V_0\,,$$

which is negative (i.e., the first excited state is a bound state) only if $2ma^2V_0/\hbar^2 > \pi^2/4$.

3. In region 1 ($0 < x < a$), $k = \sqrt{3mV/(2\hbar^2)}$; in region 2 ($x > a$), $\kappa = \sqrt{mV/(2\hbar^2)}$. And the wave function vanishes identically for $x < 0$. Imposing boundary conditions at $x = 0$, the wave function can be written as $\psi_1(x) = A\sin(kx)$ and $\psi_2(x) = B\exp(-\kappa x)$. We then need to impose boundary conditions at $x = a$:

$$A\sin(ka) = Be^{-\kappa a} \qquad \text{and} \qquad Ak\cos(ka) = -B\kappa e^{-\kappa a}\,.$$

Taking the ratio of the two equations, we obtain $\tan(ka) = -k/\kappa = -\sqrt{3}$; therefore, $ka = -\pi/3$ and $\sin(ka) = -\sqrt{3}/2$, $\cos(ka) = 1/2$. We can then use, say, the first of the two equations to solve for $B = A(\sqrt{3}/2)\exp(\kappa a)$ and obtain

$$P(x > a) = \frac{\int_a^\infty A^2(3/4)e^{2\kappa a}e^{-2\kappa x}\,dx}{\int_0^a A^2\sin^2(kx)\,dx + \int_a^\infty A^2(3/4)e^{2\kappa a}e^{-2\kappa x}\,dx} = \frac{3/(8\kappa)}{a/2 + \sqrt{3}/(8k) + 3/(8\kappa)},$$

which gives the desired result upon multiplying numerator and denominator by $24k$ and a few algebraic steps.

4. For a one-dimensional harmonic oscillator with amplitude a, we know that $x(t) = a\sin\omega t$ and $v(t) = a\omega\cos\omega t$. The classical probability is then given by:

$$P_{\mathrm{cl}}(x)dx = \frac{dx/v}{\pi/\omega} = \frac{dx}{\pi a\cos\omega t} = \frac{dx}{\pi\sqrt{a^2 - x^2}}.$$

(Note that π/ω, the half period, is the time the oscillator takes to travel from $-a$ to a.)

Normalisation can be checked for example by change of variable $x = a\cos\theta$.

The quantum probability distribution corresponding to the state given in the question is:

$$P_{\mathrm{q}}(x)dx = \frac{2}{\sqrt{\pi}}\frac{x^2}{x_0^3}\,\mathrm{e}^{-x^2/x_0^2}dx\,,$$

which is remarkably different from the classical case (as a simple sketch illustrates). The correspondence principle applies only for high energy states.

5. The wave functions of the problem in question ought to be the same as a simple harmonic oscillator for $x > 0$ and vanish identically for $x \leq 0$. Therefore, we can only retain the eigenstates of a conventional simple harmonic oscillator that vanish at the origin, i.e., the odd states:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad\qquad n = 1, 3, 5, \ldots$$

or equivalently $n = 2n' + 1$ and $E_{n'} = (2n' + 3/2)\hbar\omega$, for $n' \in \mathbb{N}$.

6. Notes about the correspondence principle should mention that: (i) quantum mechanics ought to agree with classical mechanics wherever the latter is expected to hold; (ii) in general, this is expected to hold in the high energy / high-temperature limit, or equivalently in the limit of large quantum numbers; (iii) formally, the scale at which quantum mechanical effects become relevant is set by Planck's constant h, and classical behaviour must be recovered in the limit $h \to 0$.

7. An operation $\hat{P}$ is linear if it preserves the vector space operations of f, namely multiplication by a scalar and addition. That is: $\hat{P}[\alpha f(x) + \beta g(x)] = \alpha\hat{P}[f(x)] + \beta\hat{P}[g(x)]$, for any two functions f and g in the vector space and two scalars α and β. Therefore, (a), (d), (e), (g), (h), (j) are linear operations, whereas (b), (c), (f), (i) are not.
The eigenfunctions are (for any scalars a, b):

(a) any $f(x)$;
(b) none but trivial constant functions;

(c) none but trivial constant functions;
(d) e^{ax};
(e) $\delta(x - x_0)$;
(f) ax;
(g) e^{ax} or $\cos(ax + b)$;
(h) x^a (including $a = 0$, i.e., a constant function);
(i) none but trivial constant functions;
(j) any even or odd f, i.e., s.t. $f(-x) = \pm f(x)$ (functions of definite parity).

8. If $\widehat{A}$ and $\widehat{B}$ are Hermitian, then $\widehat{A} + \widehat{B}$ is trivially Hermitian.

$c\widehat{A}$ is Hermitian if c is real.

$(\widehat{A}\widehat{B})^\dagger = \widehat{B}^\dagger \widehat{A}^\dagger = \widehat{B}\widehat{A}$ which is generally different from $\widehat{A}\widehat{B}$ unless the two operators commute.

$\widehat{A}\widehat{B} + \widehat{B}\widehat{A}$ is Hermitian.

The matrix element of the derivative operator d/dx between two states $|f\rangle$ and $|g\rangle$ is

$$\langle f|\frac{d}{dx}|g\rangle = \int f^*(x)\frac{d}{dx}g(x)\,dx\,.$$

By definition of adjoint, the matrix element of $(d/dx)^\dagger$ is the transpose conjugate of the matrix element of d/dx:

$$\begin{aligned}\langle f|\left(\frac{d}{dx}\right)^\dagger|g\rangle &= \left(\langle g|\frac{d}{dx}|f\rangle\right)^* = \left(\int g^*(x)\frac{d}{dx}f(x)\,dx\right)^* = \int g(x)\frac{d}{dx}f^*(x)\,dx \\ &= [f^*(x)g(x)]\,|_{-\infty}^{\infty} - \int f^*(x)\frac{d}{dx}g(x)\,dx\,,\end{aligned}$$

where the last line was obtained upon integrating by parts, using the relation $d(f^*g)/dx = f^*dg/dx + gdf^*/dx$. Given that the functions vanish at infinity, as the question states, we finally arrive at the relation:

$$\langle f|\left(\frac{d}{dx}\right)^\dagger|g\rangle = -\langle f|\frac{d}{dx}|g\rangle\,,$$

thus showing that d/dx is not Hermitian; it is in fact anti-Hermitian, and therefore becomes Hermitian if multiplied by the imaginary unit, such as in $-i\hbar\mathrm{d}/\mathrm{d}x$.
A similar calculation, and upon integrating by parts twice, shows that $\mathrm{d}^2/\mathrm{d}x^2$ is instead Hermitian (or more generally, for any anti-Hermitian operator, $\hat{A}^\dagger = -\hat{A}$, it is clear that A^2 is Hermitian, since $(A^2)^\dagger = \hat{A}^\dagger\hat{A}^\dagger = \hat{A}^2$).

9. Trivially, $\hat{a} = (\hat{A}^\dagger + \hat{A}) - i[i(\hat{A}^\dagger - \hat{A})]$, where $\hat{A}^\dagger + \hat{A}$ and $i(\hat{A}^\dagger - i\hat{A})$ are Hermitian.

10. In order to show mutual orthogonality, one needs to demonstrate that $\int \phi_1(x)\phi_2(x)dx = 0$ for any pair of the three functions. Notice that $x\mathrm{e}^{-x^2}$ is odd while the other two are even; therefore it is trivially orthogonal to them. The remaining orthogonality we need to check requires computing the integral:

$$\int_{-\infty}^{\infty}(4x^2 - 1)e^{-2x^2}\,dx = \sqrt{\frac{\pi}{2}} - \sqrt{\frac{\pi}{2}} = 0\,,$$

as expected.

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Possibly useful trick, thanks to the absolute convergence of a Gaussian integral:

$$\int_{-\infty}^{\infty} 4x^2 e^{-2x^2}\,dx = -2\frac{d}{da}\int_{-\infty}^{\infty} e^{-2x^2 a}\,dx\bigg|_{a=1} = -2\frac{d}{da}\sqrt{\frac{\pi}{2a}}\bigg|_{a=1} = -2\sqrt{\frac{\pi}{2}}\frac{(-1)}{2a^{1/4}}\bigg|_{a=1} = \sqrt{\frac{\pi}{2}}\,.$$

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11. For (a), by inspection, $|\psi_a\rangle \propto c|\phi_1\rangle - |\phi_2\rangle$ is orthogonal to ϕ_1. The normalisation constant is obtained by imposing $\langle\psi_a|\psi_a\rangle = 1$:

$$\begin{aligned} (c\langle\phi_1| - \langle\phi_2|)\,(c|\phi_1\rangle - |\phi_2\rangle) &= c^2 - c\langle\phi_1|\phi_2\rangle - c\langle\phi_2|\phi_1\rangle + 1 = 1 - c^2 \\ \rightarrow \qquad |\psi_a\rangle &= \frac{1}{\sqrt{1-c^2}}\,(c|\phi_1\rangle - |\phi_2\rangle)\,. \end{aligned}$$

For (b), one can proceed systematically by solving

$$(\alpha|\phi_1\rangle + \beta|\phi_2\rangle)^\dagger(|\phi_1\rangle + |\phi_2\rangle) = (\alpha+\beta)(1+c) = 0$$

to find $\beta = -\alpha$, and therefore $|\psi_b\rangle \propto |\phi_1\rangle - |\phi_2\rangle$. The normalisation constant can be found in a similar way as above,

$$|\psi_b\rangle = \frac{1}{\sqrt{2(1-c)}}\,(|\phi_1\rangle - |\phi_2\rangle)\,.$$

12. Recall from the lecture notes that

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int \phi(p) e^{ipx/\hbar}\,dp\,,$$

where $\phi(p)$ is the momentum-domain wavefunction. One can then see that the space-domain shift operation $x \to x - x_0$ corresponds to a multiplication by $\exp(-ipx_0/\hbar)$ in momentum-domain:

$$\phi(p) \to \phi(p) e^{-ipx_0/\hbar}\,.$$

This is an operation that trivially preserves the norm of $\phi(p)$.

13. Any Hermitian operator is an allowed observable of the system (however cumbersome it may be to measure it); and the sum of two Hermitian operator is Hermitian, therefore C is an observable.

Let us write C in matrix form in the basis of eigenstates of A, and then diagonalise to find its eigenvalues as well as the eigenvectors expressed as linear combinations of $u_\pm$ (which are needed for the last part of the question). We start by inverting the states in the question to find:

$$u_+ = (v_+ + v_-)/\sqrt{2} \qquad\qquad u_- = (v_+ - v_-)/\sqrt{2}\,.$$

Then, computing matrix elements for example as $\langle u_+|\hat{C}|u_-\rangle = \langle u_+|\hat{A}|u_-\rangle + [(\langle v_+| + \langle v_-|)\hat{B}(|v_+\rangle - |v_-\rangle)]/2 = 0 + 2/2 = 1$, we obtain

$$\begin{aligned}\hat{C} &= \langle u_+|\hat{C}|u_+\rangle\, |u_+\rangle\langle u_+| + \langle u_+|\hat{C}|u_-\rangle\, |u_+\rangle\langle u_-| + \langle u_-|\hat{C}|u_+\rangle\, |u_-\rangle\langle u_+| + \langle u_-|\hat{C}|u_-\rangle\, |u_-\rangle\langle u_-| \\ &= |u_+\rangle\langle u_+| + |u_+\rangle\langle u_-| + |u_-\rangle\langle u_+| - |u_-\rangle\langle u_-|\end{aligned}$$

or in matrix form

$$C = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} .$$

The corresponding secular equation $(1-\lambda)(-1-\lambda)-1 = 0$ gives the eigenvalues $\lambda = \pm\sqrt{2}$, and we can solve for the eigenvectors by solving the system of linear equations:

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \pm\sqrt{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

to obtain

$$w_\pm = \sqrt{\frac{1}{2}\left(1 \pm \frac{1}{\sqrt{2}}\right)}u_+ \pm \sqrt{\frac{1}{2}\left(1 \mp \frac{1}{\sqrt{2}}\right)}u_- .$$

Once again, we can invert these equations to find

$$u_+ = \sqrt{\frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)}w_+ + \sqrt{\frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)}w_- .$$

Therefore, following a measurement of A with outcome $+1$, the probabilities of measuring C and obtaining the values $\pm\sqrt{2}$ are $(2 \pm \sqrt{2})/4$, respectively, and

$$\langle u_+|\hat{C}|u_+\rangle = \sqrt{2}\,\frac{2+\sqrt{2}}{4} - \sqrt{2}\,\frac{2-\sqrt{2}}{4} = 1 .$$

After C is measured, the system will be in one of its eigenstates, which we already expressed in terms of u_+ and u_- earlier.

14. From the lecture notes, we know that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right) \qquad \text{and} \qquad \hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}\left(\hat{a}^\dagger - \hat{a}\right) .$$

Also, by symmetry of the system, $\langle\hat{x}\rangle = \langle\hat{p}\rangle = 0$. Therefore, all we need to compute are

$$\begin{aligned}\langle\phi_n|\hat{x}^2|\phi_n\rangle &= \frac{\hbar}{2m\omega}\langle\phi_n|\left(\hat{a}^\dagger + \hat{a}\right)^2|\phi_n\rangle \\ \langle\phi_n|\hat{p}^2|\phi_n\rangle &= -\frac{m\omega\hbar}{2}\langle\phi_n|\left(\hat{a}^\dagger - \hat{a}\right)^2|\phi_n\rangle .\end{aligned}$$

Notice that, by the properties of the number operator and of its eigenstates,

$$\begin{aligned}\langle\phi_n|\left(\hat{a}^\dagger + \hat{a}\right)^2|\phi_n\rangle &= -\langle\phi_n|\left(\hat{a}^\dagger - \hat{a}\right)^2|\phi_n\rangle \\ &= \langle\phi_n|\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger|\phi_n\rangle = \langle\phi_n|2\hat{a}^\dagger\hat{a} + 1|\phi_n\rangle = 2n+1 ,\end{aligned}$$

where we used the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$. Finally,

$$\begin{aligned}
\Delta x &= \sqrt{\langle \phi_n | \hat{x}^2 | \phi_n \rangle} = \sqrt{\frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)} \\
\Delta p &= \sqrt{\langle \phi_n | \hat{p}^2 | \phi_n \rangle} = \sqrt{m\omega\hbar\left(n + \frac{1}{2}\right)}
\end{aligned}$$

and one arrives at the desired result $\Delta x \Delta p = \hbar(n + 1/2)$.