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Solutions to Examination in Quantum Mechanics

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Also available at `http://www.teorfys.uu.se/~edsjo/kmek/index.html`.

1. a) Let A correspond to either p_x or x and let H be the Hamilton operator.

$$\frac{d\langle A\rangle}{dt} = \frac{d\left[\int \Psi^* A\Psi d^3x\right]}{dt} = \int \frac{\partial\Psi^*}{\partial t}A\Psi d^3x + \int \Psi^* A\frac{\partial\Psi}{\partial t}$$

Now use that

$$\begin{aligned} H\Psi &= i\hbar\frac{\partial\Psi}{\partial t} \\ (H\Psi)^* &= -i\hbar\frac{\partial\Psi^*}{\partial t}. \end{aligned}$$

We then get

$$\frac{d\langle A\rangle}{dt} = -\frac{1}{i\hbar}\int (H\Psi)^* A\Psi d^3x + \frac{1}{i\hbar}\int \Psi^* AH\Psi d^3x$$

and by using hermiticity of H ($V(\mathbf{r})$ real) we get

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\int \Psi^*(AH - HA)\Psi d^3x = \frac{1}{i\hbar}\int \Psi^*[A,H]\Psi d^3x.$$

To conclude we have proven that

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle [A,H]\rangle \tag{1}$$

For $A = p_x$, $H = p_x^2/2m$ we see directly that the righthand side of Eq. (1) is 0. The same is easily proven for $A = p_x$ and $H = (p_x^2 + p_y^2 + p_z^2)/2m$.
Further on, with $A = x$ and $H = (p_x^2 + p_y^2 + p_z^2)/2m + V(\mathbf{r})$ we get

$$m\frac{d\langle x\rangle}{dt} = \frac{1}{2i\hbar}\langle [x,p_x^2]\rangle + \frac{1}{2i\hbar}\langle [x,p_y^2]\rangle + \frac{1}{2i\hbar}\langle [x,p_z^2]\rangle + \frac{m}{i\hbar}\langle [x,V(\mathbf{r})]\rangle.$$

Now use that $[x, p_y^2] = 0$, $[x, p_z^2] = 0$ and $[x, V(\mathbf{r})] = 0$ and we get

$$m\frac{d\langle x\rangle}{dt} = \frac{1}{2i\hbar}\langle [x, p_x^2]\rangle = \frac{1}{2i\hbar}\langle p_x \underbrace{[x, p_x]}_{i\hbar}\rangle + \frac{1}{2i\hbar}\langle \underbrace{[x, p_x]}_{i\hbar} p_x\rangle = \langle p_x\rangle$$

With $A = p_x$ and $H = (p_x^2 + p_y^2 + p_z^2)/2m + V(\mathbf{r})$ we get

$$\begin{aligned}
\frac{d\langle p_x\rangle}{dt} &= \frac{1}{i\hbar}\langle [p_x, H]\rangle = \frac{1}{i\hbar}\langle [p_x, V(\mathbf{r})]\rangle \\
&= \frac{1}{i\hbar}\int \Psi^* \left(-i\hbar\frac{\partial V(\mathbf{r}\Psi(\mathbf{r})}{\partial x}\right) d^3x - \frac{1}{i\hbar}\int \Psi^* V(\mathbf{r}) \left(-i\hbar\frac{\partial \Psi(\mathbf{r})}{\partial x}\right) d^3x \\
&= \int \Psi^* \left(-\frac{\partial V(\mathbf{r})}{\partial x}\right) \Psi d^3x - \int \Psi^* V(\mathbf{r}) \left(-\frac{\partial \Psi}{\partial x}\right) d^3x + \int \Psi^* V(\mathbf{r}) \left(-\frac{\partial \Psi}{\partial x}\right) d^3x \\
&= \int \Psi^* \left(-\frac{\partial V(\mathbf{r})}{\partial x}\right) \Psi d^3x = \langle -\frac{\partial V(\mathbf{r})}{\partial x}\rangle.
\end{aligned}$$

Thus the Ehrenfest relations for a particle of mass m in a real potential are

$$\left\{\begin{array}{lcl} m\frac{d\langle x\rangle}{dt} & = & \langle p_x\rangle \\ \frac{d\langle p_x\rangle}{dt} & = & \langle -\frac{\partial V(\mathbf{r})}{\partial x}\rangle. \end{array}\right.$$

b) Let $\hat{A}$ be a hermitian operator and let $|i\rangle$ and $|j\rangle$ be two eigenstates of $\hat{A}$ with eigenvalues $a_i \neq a_j$, i e

$$\left\{\begin{array}{lcl} \hat{A}|i\rangle & = & a_i|i\rangle \\ \hat{A}|j\rangle & = & a_j|j\rangle \end{array}\right. \qquad a_i \neq a_j.$$

Now consider

$$\langle j|\hat{A}|i\rangle = \langle j|a_i|i\rangle = a_i\langle j|i\rangle \tag{2}$$

and then consider the same expression but let $\hat{A}$ act to the left instead,

$$\begin{aligned}
\langle j|\hat{A}|i\rangle &= \{\hat{A} \text{ hermitian}\} = \langle \hat{A}j|i\rangle = a_j^*\langle j|i\rangle \\
&= \left\{\begin{array}{l} \text{eigenvalues of a hermitian} \\ \text{operator are real} \end{array}\right\} = a_j\langle j|i\rangle.
\end{aligned} \tag{3}$$

Take Eq. (2) - Eq. (3) and we get

$$0 = (a_i - a_j)\langle j|i\rangle.$$

Since $a_i \neq a_j$ we must have

$$\langle j|i\rangle = 0,$$

i e the states $|i\rangle$ and $|j\rangle$ are orthogonal.

2. a) The time independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2}+V(x)u(x)=Eu(x) \tag{4}$$

yields

$$\begin{cases} \frac{d^2u}{dx^2}+\frac{u(x)}{a^2}=0 & , \quad x<0 \\ \frac{d^2u}{dx^2}+4\frac{u(x)}{a^2}=0 & , \quad x>0. \end{cases}$$

Now make the Ansatz

$$\begin{cases} u(x)=Ae^{ix/a}+Be^{-ix/a} & , \quad x<0 \\ u(x)=Ce^{i2x/a}+De^{-i2x/a} & , \quad x>0. \end{cases}$$

Since we don't have any reflected wave in the region $x>0$, $D=0$. Continuity of the wave function and its derivative at $x=0$ gives

$$\begin{cases} A+B=C \\ A-B=2C \end{cases}$$

from which we get

$$\begin{cases} B=-\frac{A}{3} \\ C=\frac{2A}{3} \end{cases}$$

and the wave function is thus

$$\begin{cases} u(x)=A\left[e^{ix/a}-\frac{1}{3}e^{-ix/a}\right] & , \quad x<0 \\ u(x)=\frac{2A}{3}e^{i2x/a} & , \quad x>0. \end{cases}$$

The incoming, transmitted and reflected currents are given by

$$\begin{aligned} S_{\text{inc}} &= \Re\left[-\frac{i\hbar}{m}u^*_{\text{inc}}\frac{du_{\text{inc}}}{dx}\right]=\frac{\hbar|A|^2}{ma} \\ S_{\text{trans}} &= \Re\left[-\frac{i\hbar}{m}u^*_{\text{trans}}\frac{du_{\text{trans}}}{dx}\right]=\frac{8\hbar|A|^2}{9ma} \\ S_{\text{refl}} &= \Re\left[-\frac{i\hbar}{m}u^*_{\text{refl}}\frac{du_{\text{refl}}}{dx}\right]=\frac{\hbar|A|^2}{9ma} \end{aligned}$$

The transmission and reflection coefficients are then

$$\begin{aligned} T &= \frac{S_{\text{trans}}}{S_{\text{inc}}}=\frac{8}{9} \\ R &= \frac{S_{\text{refl}}}{S_{\text{inc}}}=\frac{1}{9}. \end{aligned}$$

We note that $T+R=1$ in accordance with the conservation of the probability current density.

b) The time independent Schrödinger equation, Eq. (4), yields

$$\begin{cases} \frac{d^2u}{dx^2} + \frac{u(x)}{a^2} = 0 & , \quad x<0 \\ \frac{d^2u}{dx^2} - 2\frac{u(x)}{a^2} = 0 & , \quad x>0. \end{cases}$$

Now make the Ansatz

$$\begin{cases} u(x) = Ae^{ix/a} + Be^{-ix/a} & , \quad x<0 \\ u(x) = Ce^{-\sqrt{2}x/a} + De^{\sqrt{2}x/a} & , \quad x>0. \end{cases}$$

Since the wave function must remain finite when $x \to \infty$, $D=0$. We now want to determine A and B in terms of C (which according to the problem text is real and positive). Continuity of the wave function and its derivative at $x=0$ gives

$$\begin{cases} A+B=C \\ iA-iB=-\sqrt{2}C \end{cases}$$

from which we get

$$\begin{cases} A &= \left(\frac{1}{2}+\frac{i}{\sqrt{2}}\right)C = \frac{\sqrt{3}}{2}e^{i\alpha}C \\ B &= \left(\frac{1}{2}-\frac{i}{\sqrt{2}}\right)C = \frac{\sqrt{3}}{2}e^{-i\alpha}C \end{cases}$$

with $\alpha = \arctan\sqrt{2}$. Putting $u(0)=1$ gives the wave function

$$\begin{cases} u(x) = \sqrt{3}\cos\left(\frac{x}{a}+\alpha\right) & , \quad x<0 \\ u(x) = e^{-\sqrt{2}x/a} & , \quad x>0 \end{cases}$$

with $\alpha = \arctan\sqrt{2}$.

Note to b): That the wave function has to be real for $x<0$ if it is real for $x>0$ follows easily from the continuity equation (current conservation),

$$S_x = -\frac{i\hbar}{m}\left[u^*\frac{du}{dx} - u\frac{du^*}{dx}\right] = \text{constant}.$$

Since $u \to 0$ as $x \to \infty$ we have $S_x = 0$ which leads to

$$u^*\frac{du}{dx} - u\frac{du^*}{dx} = 0 \quad \Rightarrow \quad u^2\frac{d(u^*/u)}{dx} = 0 \quad \Rightarrow \quad u^* = F\,u$$

where the constant F is x-independent. Then if $F=1$ for $x>0$ like in this case, it must be equal to 1 also for $x<0$. Thus $u^*=u$, i e u is real for all x.

3. **a)** The norm of ψ is

$$\int \psi^* \psi d^3x = \frac{1}{64\pi a^5} \int_0^{2\pi} d\varphi \int_0^{\pi} (\sin\theta)^3 d\theta \int_0^{\infty} r^4 e^{-r/a} dr.$$

The hint and Physics Handbook yields

$$\int \psi^* \psi d^3x = \frac{1}{64\pi a^5} 2\pi \frac{8}{3!} 4! a^5 = 1$$

i e the wave function is normalized.

Let's apply $\hat{L}_z$ to ψ to get the magnetic quantum number,

$$\hat{L}_z \psi = -i\hbar \frac{\partial \psi}{\partial \varphi} = \hbar \psi.$$

Hence the magnetic quantum number is $m = 1$.

Now apply the ladder operator $\hat{L}_+$ to ψ,

$$\hat{L}_+ \psi = (\hat{L}_x + i\hat{L}_y)\psi = \hbar e^{i\varphi} \left[\frac{\partial}{\partial \theta} + i \cot\theta \frac{\partial}{\partial \varphi} \right] \psi = 0$$

since differentiation with respect to θ corresponds to a shift by a factor $\cot\theta$ and differentiation with respect to φ corresponds to a multiplication by i. Since the ladder operator $\hat{L}_+$ applied to ψ gives zero, the magnetic quantum number and the orbital angular momentum quantum number are the same and hence $l = 1$.

b) The time independent Schrödinger equation is here

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r)\psi = E\psi$$

or

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2 (r\psi)}{\partial r^2} + \frac{1}{2mr^2} \hat{L}^2 \psi + V(r)\psi - E\psi = 0$$

with $\hat{L}^2 \psi = l(l+1)\hbar^2 \psi = 2\hbar^2 \psi$. Insertion of the explicit expression for ψ gives

$$\left[-\frac{\hbar^2}{mr^2} + \frac{\hbar^2}{mar} - \frac{\hbar^2}{8ma^2} + \frac{\hbar^2}{mr^2} + V(r) - E \right] r e^{-r/2a} = 0$$

For $r > 0$ we have

$$\frac{\hbar^2}{mar} - \frac{\hbar^2}{8ma^2} + V(r) - E = 0.$$

Taking the limit as $r \to \infty$ gives

$$\begin{aligned} E &= -\frac{\hbar^2}{8ma^2} \\ V(r) &= -\frac{\hbar^2}{mar} \end{aligned}$$

c) The probability current density is given by

$$\mathbf{S} = \Re\left[\psi^* \left(-\frac{i\hbar}{m}\right) \nabla\psi\right].$$

Notice that

$$-i\hbar\nabla\psi = -i\hbar\frac{1}{r}\frac{1}{\sin\theta}\frac{\partial\psi}{\partial\varphi} + \cdots$$

where in this case

$$-i\hbar\frac{\partial\psi}{\partial\varphi} = \hbar\psi$$

and where the terms $+\cdots$ don't contribute to $\mathbf{S}$. Hence we obtain

$$\mathbf{S} = \frac{\hbar}{m}\mathbf{e}_\varphi\psi^*\frac{1}{r\sin\theta}\psi = \frac{\hbar}{64\pi m a^5} r e^{-r/a}\sin\theta\,\mathbf{e}_\varphi.$$

The total probability current density through the half plane $\varphi = 0$ is

$$\begin{aligned} S_{\text{tot}} &= \mathbf{e}_\varphi \cdot \int_0^\pi \left(\int_0^\infty \mathbf{S} r dr\right) d\theta = \frac{\hbar}{64\pi m a^5}\int_0^\infty r^2 e^{-r/a} dr \int_0^\pi \sin\theta d\theta \\ &= \frac{\hbar}{16\pi m a^2} = \frac{\hbar^2}{8ma^2}\frac{1}{2\pi\hbar} = \frac{|E|}{h}. \end{aligned}$$

This result seems satisfactory since the total probability current has dimension 1/time, i e the dimension of a frequency as it should.

4. a) Since $\psi^*\psi$ is even, x is odd and we integrate over a symmetric interval we can immediately conclude that

$$\langle x\rangle = 0.$$

Hence

$$\begin{aligned} (\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = \langle x^2\rangle &= \frac{3}{2a^3}\int_{-a}^a x^2(a-|x|)^2 dx = \frac{3}{a^3}\int_0^a x^2(a-x)^2 dx \\ &= \frac{3}{a^3}\int_0^a \left(x^2a^1 - 2ax^3 + x^4\right) dx = 3a^2\left(\frac{1}{3} - \frac{1}{2} + \frac{1}{5}\right) = \frac{a^2}{10} \end{aligned}$$

which gives

$$\Delta x = \frac{a}{\sqrt{10}}.$$

b) The wave function in momentum space is given by

$$\begin{aligned} \phi(p_x) &= \sqrt{\frac{3}{4\pi\hbar a^3}}\int_{-a}^a e^{ip_x x/\hbar}(a-|x|)dx = \sqrt{\frac{3}{\pi\hbar a^3}}\int_0^a \cos\left(\frac{p_x x}{\hbar}\right)(a-x)dx \\ &= \sqrt{\frac{3\hbar}{\pi a^3}}\left[\frac{1}{p_x}\sin\left(\frac{p_x x}{\hbar}\right)(a-x)\right]_0^a + \sqrt{\frac{3\hbar}{\pi a^3}}\int_0^a \frac{1}{p_x}\sin\left(\frac{p_x x}{\hbar}\right)dx \\ &= \sqrt{\frac{3\hbar}{\pi a^3}}\frac{1-\cos\left(\frac{p_x a}{\hbar}\right)}{p_x^2}. \end{aligned}$$

Since $\phi^*\phi$ is even and p_x is odd we can immediately conclude

$$\langle p_x \rangle = 0.$$

Thus we have

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 = \langle p_x^2 \rangle = \frac{3\hbar^3}{\pi a^3}\int_{-\infty}^{\infty} \frac{\left[1-\cos\left(\frac{p_x a}{\hbar}\right)\right]^2}{p_x^2} dp_x = \frac{3\hbar^2}{a^2}$$

which gives

$$\Delta p_x = \frac{\sqrt{3}\hbar}{a}.$$

c) We get

$$\Delta x \Delta p_x = \sqrt{\frac{3}{10}}\hbar > \frac{1}{2}\hbar.$$

Hence the uncertainty product is somewhat larger than that of a minimum uncertainty wave packet as expected.

Note on b): Alternatively $(\Delta p_x)^2$ can be calculated as

$$\begin{aligned}(\Delta p_x)^2 &= \int_{-\infty}^{\infty} \psi^* \hat{p}_x^2 \psi dx = \int_{-\infty}^{\infty} (\hat{p}_x\psi)^* \hat{p}_x \psi dx \\ &= \frac{3}{2a^3}\int_{-a}^{0} (-i\hbar)^*(-i\hbar)dx + \frac{3}{2a^3}\int_{0}^{a} (i\hbar)^*(i\hbar)dx = \frac{3\hbar^2}{a^2}\end{aligned}$$

5. **a)** The problem considered is governed by the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + mgx\psi(x) = E\psi(x) \quad , \quad x > 0 \tag{5}$$

with boundary conditions $\psi(0) = 0$ and $\psi(x) \to 0$ as $x \to \infty$ since the probability is zero to find the particle in the region $x < 0$ as well as very far away on the positive x-axis. According to the hints, Eq. (5) has the solution (apart from normalization)

$$\psi(x) = z^{1/3}\left(J_{-1/3}(z) + J_{1/3}(z)\right) \quad \text{with } z = \beta(E - mgx)^{3/2} \text{ and } \beta = \frac{2\sqrt{2}}{3g\hbar\sqrt{m}}$$

where $J_\mu(z)$ denotes a Bessel function of order μ.
For $x > E/mg$, ψ can also be expressed as essentially a modified Bessel function,

$$\psi(x) = \frac{\sqrt{3}}{\pi}|z|^{1/3}K_{1/3}(|z|).$$

which tends to zero as $x \to +\infty$. Any other linearly independent solution of the original differential equation (5) tends to ∞ as $x \to \infty$ and hence the solution given in the hint is (as for normalization) *the* solution which fulfills the boundary condition at infinity. For $x < E/mg$ (and not too close to the *classical turning point* E/mg), ψ may be approximated by[1]

$$\psi(x) \simeq C\cos\left(\beta(E-mgx)^{3/2} - \frac{\pi}{4}\right) \quad , x \text{ less than and not too close to } E/mg. \tag{6}$$

The remaining boundary condition $\psi(0) = 0$ determines the energy eigenvalues E_k:

$$\begin{aligned}
&\cos\left(\beta E_k^{3/2} - \frac{\pi}{4}\right) = 0 \\
&\Rightarrow \quad \beta E_k^{3/2} - \frac{\pi}{4} = \left(k + \frac{1}{2}\right)\pi \\
&\Rightarrow \quad E_k^{3/2} = \frac{k + \frac{3}{4}}{\beta} \quad k = 0, 1, 2, \ldots \\
&\Rightarrow \quad E_k = \left[\frac{k + \frac{3}{4}}{\beta}\right]^{2/3} \quad , \quad \beta = \frac{2\sqrt{2}}{3g\hbar\sqrt{m}} \quad , \quad k = 0, 1, 2, \ldots
\end{aligned}$$

b) The problem considered is governed by the differential equation

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + mgx\psi(x) = E\psi(x) & , \quad x > 0 \\ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - mgx\psi(x) = E\psi(x) & , \quad x < 0 \end{cases} \tag{7}$$

with boundary conditions $\psi(x) \to 0$ as $x \to \pm\infty$. Since we here consider bound states in a symmetric potential the eigenfunctions have either *even parity* or *odd parity* and we need only consider $x > 0$ when solving the Schrödinger equation (7). Due to the continuity condition at $x = 0$, the odd parity wave functions have $\psi(0) = 0$ and hence we have already determined the eigenvalues in a). The even parity wave functions with energy eigenvalues E_p have $\psi'(0) = 0$ and hence using Eq. (6) in a) (and regarding C as a constant) we obtain

$$\begin{aligned}
&\sin\left(\beta E_p^{3/2} - \frac{\pi}{4}\right) = 0 \\
&\Rightarrow \quad \beta E_p^{3/2} - \frac{\pi}{4} = p\pi \quad , \quad p = 0, 1, 2, \ldots \\
&\Rightarrow \quad E_p^{3/2} = \frac{p + \frac{1}{4}}{\beta}\pi \quad , \quad p = 0, 1, 2, \ldots \\
&\Rightarrow \quad E_p = \left[\frac{p + \frac{1}{4}}{\beta}\pi\right]^{2/3} \quad , \quad \beta = \frac{2\sqrt{2}}{3g\hbar\sqrt{m}} \quad , \quad p = 0, 1, 2, \ldots
\end{aligned}$$

We can write the energy eigenvalues as

$$E_n = \left[\frac{n + \frac{1}{2}}{2\beta}\pi\right]^{2/3} \quad , \quad \beta = \frac{2\sqrt{2}}{3g\hbar\sqrt{m}} \quad , \quad n = 0, 1, 2, \ldots$$

where even n correspond to even parity and odd n correspond to odd parity. These approximate eigenvalues are actually quite decent, the error in the ground state energy being less than 10% and the errors in the excited energies all being less than 1%.

[1] Eq. (6) actually follows directly from the exact solution and the asymptotic formula for the Bessel function on page 202 in Mathematics Handbook, a formula which is quite accurate for low orders of the Bessel function such as $\pm 1/3$ even when the argument is rather moderate.