F3EMPS & MN
Staffan Yngve

Institutionen för teoretisk fysik

# Solutions to Examination in Quantum Mechanics

**12 January 1996**

Solutions made mainly by Staffan Yngve and partly by Joakim Edsjö

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

**1.** If $\Psi(x)$ is normalized, $\int \Psi^* \Psi d^3 r = 1$, the expectation value of $A$ is given by

$$\langle A \rangle = \int \Psi^* A \Psi d^3 x$$

If $\psi_n$ is a complete set of orthonormal eigenfunctions of $A$ we have

$$A\psi_n = A_n \psi_n$$

$$\int \psi_m^* \psi_n d^3 r = \begin{cases} 0 & , \quad n \neq m \\ 1 & , \quad n = m \end{cases}$$

and $\Psi$ can then (at a certain time) be expanded in $\psi_n$,

$$\Psi = \sum_n c_n \psi_n .$$

We then get

$$\begin{aligned} 1 = \int \Psi^* \Psi d^3 r &= \int \left( \sum_m c_m \psi_m \right)^* \left( \sum_n c_n \psi_n \right) d^3 r = \sum_{m,n} c_m^* c_n \int \psi_m^* \psi_n d^3 r \\ &= \sum_{m,n} c_m^* c_n \delta_{mn} = \sum_n c_n^* c_n = \sum_n |c_n|^2 \\ &\Rightarrow \sum_n |c_n|^2 = 1 \end{aligned}$$

and

$$\begin{aligned} \langle A \rangle = \int \Psi^* A \Psi d^3 r &= \int \left( \sum_m c_m \psi_m \right)^* A \left( \sum_n c_n \psi_n \right) d^3 r \\ &= \int \left( \sum_m c_m \psi_m \right)^* \left( \sum_n c_n A \psi_n \right) d^3 r \int \left( \sum_m c_m \psi_m \right)^* \left( \sum_n c_n A_n \psi_n \right) d^3 r \\ &= \sum_{m,n} c_m^* c_n A_n \int \psi_m^* \psi_n d^3 r = \sum_{m,n} c_m^* c_n A_n \delta_{mn} = \sum_n c_n^* c_n A_n = \sum_n |c_n|^2 A_n \end{aligned}$$

If we don't have degeneration, $|c_n|^2$ is the probability to obtain the value $A_n$ of the state (at a certain time) given by $\Psi$. In case of degeneration, the probability to obtain the value $A_n$ is given by $\sum_n' |c_n|^2$ where we in $\sum'$ sum over all states corresponding to the value $A_n$.

**2.** See Bransden & Joachain, pages 114–115.

**3.** Let $B$ correspond to either $p_x$ or $x$ and let $H$ be the Hamilton operator. We then get

$$\frac{d\langle B\rangle}{dt} = \frac{d\int \Psi^* B\Psi d^3r}{dt} = \int \left(\frac{\partial \Psi^*}{\partial t}\right) B\Psi d^3r + \int \Psi^* \underbrace{\frac{\partial B}{\partial t}}_{0} \Psi d^3r + \int \Psi B \left(\frac{\partial \Psi}{\partial t}\right) d^3r$$

where $\partial B/\partial t$ is 0 since neither the *operator* $p_x$ nor $x$ depend on time. Now use the Schrödinger equation

$$\begin{cases} H\Psi &= i\hbar\frac{\partial\Psi}{\partial t} \\ H\Psi^* &= -i\hbar\frac{\partial\Psi^*}{\partial t} \end{cases}$$

and we get

$$\begin{aligned} \frac{d\langle B\rangle}{dt} &= -\frac{1}{i\hbar}\int H\Psi^* B\Psi d^3r + \frac{1}{i\hbar}\int \Psi^* BH\Psi d^3r = \{H \text{ is hermitian}\} \\ &= \frac{1}{i\hbar}\int \Psi^*(BH - HB)\Psi d^3r = \frac{1}{i\hbar}\int \Psi^*[B,H]\Psi d^3r \end{aligned}$$

i.e.

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

With $B = x$, $H = (\mathbf{p} - q\mathbf{A})^2/2m$ and $\mathbf{A}(\mathbf{r}) = A_x(y,z)\mathbf{e}_x$ we then get

$$\begin{aligned} m\frac{d\langle x\rangle}{dt} &= \frac{1}{i\hbar}\langle [x,(p_x - qA_x)^2]\rangle \\ &= \frac{1}{i\hbar}\langle (p_x - qA_x)[x,(p_x - qA_x)]\rangle + \frac{1}{i\hbar}\langle [x,(p_x - qA_x)](p_x - qA_x)\rangle. \end{aligned}$$

Since $A_x$ doesn't depend on $x$ we get

$$[x,(p_x - qA_x)] = \underbrace{[x,p_x]}_{i\hbar} - q\underbrace{[x,A_x]}_{0} = i\hbar$$

which finally gives

$$m\frac{d\langle x\rangle}{dt} = \langle (p_x - qA_x)\rangle.$$

For $B = p_x$, $H = (\mathbf{p} - q\mathbf{A})^2/2m$ and $\mathbf{A}(\mathbf{r}) = A_x(y,z)\mathbf{e}_x$ we get

$$\frac{d\langle p_x\rangle}{dt} = \frac{1}{2mi\hbar}\langle [p_x,(\mathbf{p} - qA_x\mathbf{e}_x)^2]\rangle = \frac{1}{2mi\hbar}\langle [p_x,(p_x - qA_x)^2]\rangle = 0$$

**4.** The time independent Schrödinger equation,

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

is in this case

$$\left\{ \begin{array}{lll} \frac{d^2u}{dx^2} + \frac{2mE}{\hbar^2}u(x) = 0 & , & x < 0 \text{ and } x > a \\ \frac{d^2u}{dx^2} + \left(\frac{2mE}{\hbar^2} + \frac{\eta^2}{a^2}\right)u(x) = 0 & , & 0 < x < a \end{array} \right. \tag{1}$$

For convenience, define

$$\left\{ \begin{array}{lll} k^2 & = & \frac{2mE}{\hbar^2} \\ K^2 & = & \frac{2mE}{\hbar^2} + \frac{\eta^2}{a^2} \end{array} \right.$$

which puts Eq. (1) into the form

$$\left\{ \begin{array}{lll} \frac{d^2u}{dx^2} + k^2u(x) = 0 & , & x < 0 \text{ and } x > a \\ \frac{d^2u}{dx^2} + K^2u(x) = 0 & , & 0 < x < a \end{array} \right. . \tag{2}$$

Eq. (2) has the solution

$$\left\{ \begin{array}{lllll} u(x) & = & Ae^{ikx} + Be^{-ikx} & , & x < 0 \\ u(x) & = & Be^{iKx} + Ce^{-iKx} & , & 0 < x < a \\ u(x) & = & Fe^{ikx} + Ge^{-ikx} & , & x > a \end{array} \right. .$$

Since we don't have any reflected wave for $x > a$, we must have $G = 0$. Continuity of the wave function and its derivative at $x = 0$ yields

$$\left\{ \begin{array}{l} A + B = C + D \\ A - B = \frac{K}{k}(C - D) \end{array} \right.$$

which subtracted by each other gives

$$2B = C\left(1 - \frac{K}{k}\right) + D\left(1 + \frac{K}{k}\right). \tag{3}$$

Continuity of the wave function and its derivative at $x = a$ yields

$$\left\{ \begin{array}{l} Ce^{iKa} + De^{-iKa} = Fe^{ika} \\ \frac{K}{k}\left(Ce^{iKa} - De^{-iKa}\right) = Fe^{ika} \end{array} \right.$$

which together gives

$$Ce^{iKa} + De^{-iKa} = \frac{K}{k}\left(Ce^{iKa} - De^{-iKa}\right). \tag{4}$$

When we have total transmission there is no reflection and hence $B = 0$ in this case. According to Eq. (3) we then have

$$D = C\frac{-1 + \frac{K}{k}}{1 + \frac{K}{k}}$$

which together with Eq. (4) gives

$$\left(1-\frac{K^2}{k^2}\right)e^{iKa}=\left(1-\frac{K^2}{k^2}\right)e^{-iKa}.$$

Since $k=K$ is an uninteresting case we get

$$\begin{aligned}
&e^{iKa}=e^{-iKa}\\
&\quad\Rightarrow\quad \sin Ka=0\\
&\quad\Rightarrow\quad Ka=n\pi \quad , \quad n=\text{integer}\\
&\quad\Rightarrow\quad K^2=\frac{n^2\pi^2}{a^2} \quad , \quad n=\text{integer}\\
&\quad\Rightarrow\quad \frac{2mE}{\hbar^2}+\frac{\eta^2}{a^2}=\frac{n^2\pi^2}{a^2} \quad , \quad n=\text{integer}\\
&\quad\Rightarrow\quad \frac{2mE}{\hbar^2}=\frac{n^2\pi^2-\eta^2}{a^2} \quad , \quad n=\text{integer}\\
&\quad\Rightarrow\quad E=\frac{\hbar^2(n^2\pi^2-\eta^2)}{2ma^2} \quad , \quad n=\text{integer}
\end{aligned}$$

i.e. for energies

$$E=\frac{\hbar^2(n^2\pi^2-\eta^2)}{2ma^2} \quad , \quad n=\text{integer such that } E>0$$

we get total transmission.

**5.** a) The expectation value $\langle r\rangle$ is given by

$$\begin{aligned}
\langle r\rangle &= N^2\int_0^{2\pi}d\phi\int_0^{\pi}(\sin\theta)^{2l+1}d\theta\int_0^{\infty}r^{2l+3}e^{-\frac{2r}{(l+1)a}}dr=\{\text{hint}\}\\
&= N^2 2\pi\frac{2^{2l+1}(l!)^2}{(2l+1)!}(2l+3)!a^{2l+4}\frac{(l+1)^{2l+4}}{2^{2l+4}}\\
&= \frac{1}{\pi(l+1)^{2l+4}(l!)^2a^{2l+3}}2\pi(l!)^2(2l+3)(2l+2)a^{2l+4}(l+1)^{2l+4}(l+1)^{2l+4}\frac{1}{8}\\
&= a(l+1)\left(l+\frac{3}{2}\right)
\end{aligned}$$

b) The probability current density is given by

$$\mathbf{S}=\frac{\hbar}{m}\Im\left[\Psi^*\nabla\Psi\right].$$

Note that only the differentiation with respect to $\phi$ gives an imaginary contribution in this case. Hence we get

$$\mathbf{S}=\frac{\hbar}{m}\mathbf{e}_\phi\Im\left[\Psi^*\frac{1}{r\sin\theta}\frac{\partial\Psi}{\partial\phi}\right]=\frac{\hbar}{m}\mathbf{e}_\phi lN^2r^{2l-1}e^{-\frac{2r}{(l+1)a}}(\sin\theta)^{2l-1}$$

The asked for probability current through the half plane $\phi = 0$ is then given by

$$
\begin{aligned}
S_{\phi=0} &= \mathbf{e}_\phi \cdot \int_0^\pi \left( \int_0^\infty \mathbf{S} r dr \right) d\theta = \frac{\hbar}{m} l N^2 \int_0^\infty r^{2l} e^{-\frac{2r}{(l+1)a}} dr \int_0^\pi (\sin\theta)^{2l-1} d\theta \\
&= \frac{\hbar}{m} l N^2 (2l)! a^{2l+1} (l+1)^{2l+1} 2^{-2l-1} 2^{2l-1} \frac{[(l-1)!]^2}{(2l-1)!} \\
&= \frac{\hbar}{m} l \frac{1}{\pi (l+1)^{2l+4} (l!)^2 a^{2l+3}} (2l)! a^{2l+1} (l+1)^{2l+1} 2^{-2l-1} 2^{2l-1} \frac{[(l-1)!]^2}{(2l-1)!} \\
&= \frac{\hbar}{2\pi m (l+1)^3 a^2} = \frac{\omega}{2\pi}
\end{aligned}
$$

with

$$\omega = \frac{\hbar}{m(l+1)^3 a^2} = \frac{1}{\hbar} \frac{dE}{dl}.$$

One can show that $\omega / 2\pi$ the semi classical frequency.

**6.** We have the time independent Schrödinger equation

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

with

$$V(x) = \begin{cases} \infty & , \quad x < 0 \\ mgx & , \quad x > 0 \end{cases}$$

which thus gives us the equation

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

with the boundary condition $\psi(0) = 0$. We now seek a suitable dimensionless position variable and note that $2m^2 gx/\hbar^2$ has dimension 1/length$^2$, i.e. $2m^2 g/\hbar^2$ has dimension 1/length$^3$. Thus

$$X = x \left( \frac{2m^2 g}{\hbar^2} \right)^{1/3}$$

is dimensionless. Let

$$u(X) = \psi(x) \left( \frac{2m^2 g}{\hbar^2} \right)^{2/3}$$

and Eq. (5) can then be written

$$\frac{d^2 u}{dX^2} - Xu = -\frac{2mE}{\hbar^2} \left( \frac{2m^2 g}{\hbar^2} \right)^{-2/3} u.$$

Now introduce

$$\alpha = \left(\frac{2}{m\hbar^2 g^2}\right)^{1/3} E$$

and we get

$$\frac{d^2u}{dX^2} + (\alpha - X)u(X) = 0.$$

According to the hint, Eq. () has for $X < \alpha$ (but not too close to $\alpha$) the approximate solution

$$u \simeq \frac{2\sqrt{\pi}}{(\alpha - X)^{1/4}} \cos\left[\frac{2(\alpha - X)^{3/2}}{3} - \frac{\pi}{4}\right].$$

The boundary condition $u(0) = 0$ now gives

$$\begin{aligned}
\frac{2\alpha^{3/2}}{3} - \frac{\pi}{4} = \left(n + \frac{1}{2}\right)\pi \quad &, \quad n = 0, 1, 2, \ldots \\
\Rightarrow \quad \frac{2\alpha^{3/2}}{3} = \left(n + \frac{3}{4}\right)\pi \quad &, \quad n = 0, 1, 2, \ldots \\
\Rightarrow \quad \alpha^{3/2} = \left(\frac{3n}{2} + \frac{9}{8}\right)\pi \quad &, \quad n = 0, 1, 2, \ldots \\
\Rightarrow \quad \alpha_n = \left[\left(\frac{3n}{2} + \frac{9}{8}\right)\pi\right]^{2/3} \quad &, \quad n = 0, 1, 2, \ldots
\end{aligned}$$

where $E_n$ then is given by

$$E_n = \left(\frac{m\hbar^2 g^2}{2}\right)^{1/3} \alpha_n = \left(\frac{m\hbar^2 g^2}{2}\right)^{1/3} \left[\left(\frac{3n}{2} + \frac{9}{8}\right)\pi\right]^{2/3} \quad , \quad n = 0, 1, 2, \ldots$$

**Alternative solution.** Alternatively, one can go to momentum space instead. The Fourier transform of $\phi(p)$,

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

and the Schrödinger equation in the momentum representation (by formally putting $x = i\hbar\frac{d}{dp}$),

$$\frac{p^2}{2m}\phi(p) + i\hbar m g \phi(p) = E\phi(p)$$

or

$$i\hbar\frac{\phi'(p)}{\phi(p)} = \frac{p^2}{2m^2 g} - \frac{E}{mg}.$$

Integration yields

$$i\hbar \ln\phi(p) = \frac{p^3}{6m^2 g} - \frac{Ep}{mg} + \text{constant}$$

where, by a suitable choice of the integration constant, we get

$$\psi(x) = \int_{-\infty}^{\infty} e^{-i\left(\frac{p^3}{6\hbar m^2 g} - \frac{Ep}{mg\hbar}\right)} e^{ipx/\hbar} dp.$$

The boundary condition $\psi(0) = 0$ gives

$$\int_{-\infty}^{\infty} e^{i\left(\frac{Ep}{mg\hbar} - \frac{p^3}{6m^2 g\hbar}\right)} dp = 0$$

or

$$\int_{-\infty}^{\infty} \cos\left[\frac{Ep}{mg\hbar} - \frac{p^3}{6m^2 g\hbar}\right] dp = 0.$$

This integral is recognized in the hint with $X = 0$ and

$$\begin{cases} w^3 &= \frac{p^3}{2m^2 g\hbar} \\ \alpha &= \left(\frac{2}{g^2\hbar^2 m}\right)^{1/3} E \end{cases}$$

If the integral is replaced by its approximate value we get the same solutions as before.

**Note.** One can show that the approximation that is done only contributes to 0.76% error in the ground state energy and very small errors (1 per mille or less) for the higher states. The model is for example used in quark confinement and the disagreement between the model and reality should then be larger than the analytical approximation error.