Solved selected problems of An Introduction to Quantum Theory by Keith Hannabuss

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Chapter 2 - Wave Mechanics

Solution. 2.1 Let a sodium atom with a mass of $3.82 \times 10^{-26}\ kg$ emit a photon with a wavelength of $5.89 \times 10^{-7}\ m$.

From De Broglie observations the momentum of the emitted photon is $|\boldsymbol{p}| = \hbar|\boldsymbol{k}|$ where $|\boldsymbol{k}| = 2\pi/\text{wavelength}$ hence in this case

$$|\boldsymbol{k}| = \frac{2\pi}{5.89 \times 10^{-7}\ m} = 10667547.21\ m^{-1}$$

And

$$|\boldsymbol{p}| = 1.0546 \times 10^{-34}\ Js \cdot 10667547.21\ m^{-1} = 1.1249 \times 10^{-27}\ kgm/s$$

Also, we know that $|\boldsymbol{p}| = mv$ so if we assume that the sodium atom was at rest, and we use the conservation of momentum, then the velocity of recoil is given by

$$v = \frac{|\boldsymbol{p}|}{m} = \frac{1.1249 \times 10^{-27}\ kgm/s}{3.82 \times 10^{-26}\ kg} = 0.0294\ m/s$$

$\square$

Solution. 2.2 Schrödinger's time-independent equation for a particle moving in one dimension with energy E is

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

In this case, the particle is under the influence of a constant potential $V(x)=V_0$ in the interval $[0,a]$. To avoid problems at the endpoints we make ψ vanish there, hence we get that

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}=(E-V_0)\psi$$

For $x\in(0,a)$ and the boundary conditions $\psi(0)=0=\psi(a)$.
If we assume that $E>0$ then the general solution of the differential equation is

$$\psi(x)=A\cos\Big(\sqrt{2m(E-V_0)}x/\hbar\Big)+B\sin\Big(\sqrt{2m(E-V_0)}x/\hbar\Big)$$

The condition $\psi(0)=0$ implies that A must be zero.
On the other hand, the condition $\psi(a)=0$ is satisfied if

$$\sqrt{2m(E-V_0)}/\hbar=n\pi/a$$

For some integer n, then the possible energies are

$$\begin{aligned}2m(E_n-V_0)&=\frac{n^2\pi^2\hbar^2}{a^2}\\E_n&=V_0+\frac{n^2\pi^2\hbar^2}{2ma^2}\end{aligned}$$

□

Solution. 2.3 Let a particle of mass m move in the rectangle $[0,a] \times [0,b]$ in the xy-plane under the influence of a zero potential. The Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

If we assume that $\psi(x,y)$ is a product of two functions $\psi(x,y) = X(x)Y(y)$ then we can write it as

$$-\frac{\hbar^2}{2m}\left(Y\frac{\partial^2 X}{\partial x^2} + X\frac{\partial^2 Y}{\partial y^2}\right) = EXY$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\right) = E$$

Where we divided by XY. Then we see that the first and second term on the left side must be equal to a constant i.e.

$$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = \alpha \qquad -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = \beta$$

So we get that

$$-\frac{\hbar^2}{2m}\frac{\partial^2 X}{\partial x^2} = \alpha X \qquad -\frac{\hbar^2}{2m}\frac{\partial^2 Y}{\partial y^2} = \beta Y$$

From the one-dimmensional square well we know that the solution to these differential equations is

$$X = A\sin(j\pi x/a) \qquad Y = B\sin(k\pi y/b)$$

Where $\sqrt{2m\alpha}/\hbar = j\pi/a$ and $\sqrt{2m\beta}/\hbar = k\pi/b$. Also, we used that the boundary conditions are $\psi(0) = \psi(a) = \psi(b) = 0$ and we defined j,k integers. Then we have that

$$\alpha = \frac{j^2\pi^2\hbar^2}{2ma^2} \qquad \beta = \frac{k^2\pi^2\hbar^2}{2mb^2}$$

But we said that $\alpha + \beta = E$ hence the permitted energies of the system are

$$E_{j,k} = \frac{j^2\pi^2\hbar^2}{2ma^2} + \frac{k^2\pi^2\hbar^2}{2mb^2} = \frac{\pi^2\hbar^2}{2m}\left(\frac{j^2}{a^2} + \frac{k^2}{b^2}\right)$$

Let now $a = b$ then the wave function becomes

$$\psi(x,y) = C\sin(j\pi x/a)\sin(k\pi y/a)$$

Where we renamed $AB = C$. Applying the normalization condition then we have that

$$|C|^2\int_0^a\int_0^a \sin^2(j\pi x/a)\sin^2(k\pi y/a)\;dxdy = 1$$

$$|C|^2\frac{a}{2}\int_0^a \sin^2(k\pi y/a)\;dy = 1$$

$$C = \frac{2}{a}$$

Hence

$$\psi(x,y) = \frac{2}{a}\sin(j\pi x/a)\sin(k\pi y/a)$$

But since we are considering an energy of $5\pi^2\hbar^2/2ma^2$ then using the equation for $E_{j,k}$ must be that $j = 1$ and $k = 2$ or $j = 2$ and $k = 1$.
Therefore the two normalized wave functions corresponding to the energy $5\pi^2\hbar^2/2ma^2$ are

$$\begin{aligned}
\psi_{1,2}(x,y) &= \frac{2}{a}\sin(\pi x/a)\sin(2\pi y/a) \\
\psi_{2,1}(x,y) &= \frac{2}{a}\sin(2\pi x/a)\sin(\pi y/a)
\end{aligned}$$

Finally, the probability that the particle lies in the region

$$S = \{(x,y) \in \mathbb{R} : x \leq y\}$$

in each case can be computed by integration as follows

$$\begin{aligned}
\int_S |\psi_{1,2}(x,y)|^2 \; dxdy &= \frac{4}{a^2}\int_0^a \int_0^y \sin^2(\pi x/a)\sin^2(2\pi y/a) \; dxdy \\
&= \frac{4}{a^2}\int_0^a \left[\frac{y}{2} - \frac{a\sin(2\pi y/a)}{4\pi}\right]\sin^2(2\pi y/a) \; dy \\
&= \frac{1}{\pi a^2}\int_0^a 2\pi y\sin^2(2\pi y/a) - a\sin^3(2\pi y/a) \; dy \\
&= \frac{1}{\pi a^2}\left[\frac{\pi a^2}{2} - 0\right] \\
&= \frac{1}{2}
\end{aligned}$$

And

$$\begin{aligned}
\int_S |\psi_{2,1}(x,y)|^2 \; dxdy &= \frac{4}{a^2}\int_0^a \int_0^y \sin^2(2\pi x/a)\sin^2(\pi y/a) \; dxdy \\
&= \frac{4}{a^2}\int_0^a \left[\frac{y}{2} - \frac{a\sin(4\pi y/a)}{8\pi}\right]\sin^2(\pi y/a) \; dy \\
&= \frac{1}{2\pi a^2}\int_0^a 4\pi y\sin^2(\pi y/a) - a\sin(4\pi y/a)\sin^2(\pi y/a) \; dy \\
&= \frac{1}{2\pi a^2}\left[\pi a^2 - 0\right] \\
&= \frac{1}{2}
\end{aligned}$$

$\square$

Solution. 2.4 Let a particle of mass m move within a ball of radius $a \in \mathbb{R}^3$ under the influence of the potential $V(r) = 0$. Then Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

Let us take a wave function $\psi(r)$ independent of the angles then the equation in spherical coordinates become

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) = E\psi$$

But since

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) = 2r\frac{\partial\psi}{\partial r} + r^2\frac{\partial^2\psi}{\partial r^2} = r\frac{\partial^2(r\psi)}{\partial r^2}$$

We get that

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2(r\psi)}{\partial r^2} = E\psi$$

Or

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

This equation is the same equation we solved for the square well for which we know that the solution is

$$r\psi(r) = A\cos\left(\sqrt{2mE}r/\hbar\right) + B\sin\left(\sqrt{2mE}r/\hbar\right)$$

We see that at $r = 0$ we get that $r\psi(0) = 0 \cdot \psi(0) = 0$ and we know that $\psi(a) = 0$ then $r\psi(a) = 0$ so the boundary conditions are the same as the ones used for the square well so the general solution is

$$\psi(r) = \frac{B}{r}\sin(n\pi r/a)$$

Where we used that the boundary condition at a is satisfied if $\sqrt{2mE}/\hbar = n\pi/a$. Then the energies satisfying the equation are

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

Now we apply the normalization condition to determine B as follows

$$\begin{aligned}
1 &= |B|^2\int_0^{2\pi}\int_0^{\pi}\int_0^{a}\frac{\sin^2(n\pi r/a)}{r^2}r^2\sin\theta\ drd\theta d\phi \\
&= |B|^2\int_0^{2\pi}\int_0^{\pi}\int_0^{a}\sin^2(n\pi r/a)\sin\theta\ drd\theta d\phi \\
&= |B|^2\frac{a}{2}\int_0^{2\pi}\int_0^{\pi}\sin\theta\ d\theta d\phi \\
&= 2\pi a|B|^2
\end{aligned}$$

Then $B = 1/\sqrt{2\pi a}$, and hence the general solution is

$$\psi(r) = \frac{1}{r\sqrt{2\pi a}} \sin(n\pi r/a)$$

Finally, the probability of finding the particle within a distance $\frac{1}{2}a$ is given by

$$\begin{aligned}
\int |\psi(r)|^2 \, dV &= \int_0^{2\pi} \int_0^{\pi} \int_0^{a/2} \frac{\sin^2(n\pi r/a)}{2\pi a r^2} r^2 \sin\theta \; dr d\theta d\phi \\
&= \frac{1}{2\pi a} \int_0^{2\pi} \int_0^{\pi} \int_0^{a/2} \sin^2(n\pi r/a) \sin\theta \; dr d\theta d\phi \\
&= \frac{1}{2\pi a} \frac{a}{4} \int_0^{2\pi} \int_0^{\pi} \sin\theta \; d\theta d\phi \\
&= \frac{1}{8\pi} 4\pi \\
&= \frac{1}{2}
\end{aligned}$$

$\square$

Solution. 2.5

We know that the mean position of the particle on the z axis is computed as

$$\int_{-\infty}^{\infty} z|\psi(r)|^2 \; dV$$

Then using that $\psi(r)$ vanishes at the boundaries we get that

$$\int_{-\infty}^{\infty} z|\psi(r)|^2 \; dV = \int_0^a \int_0^{2\pi} \int_0^{\pi} r\cos\theta \frac{\sin^2(n\pi r/a)}{2\pi a r^2} r^2 \sin\theta \; d\theta d\phi dr = 0$$

Where we used that $\int_0^{\pi} \cos\theta \sin\theta \; d\theta = 0$.

In the same way, for $x = r\sin\theta\cos\phi$ we have that

$$\int_{-\infty}^{\infty} x|\psi(r)|^2 \; dV = \int_0^a \int_0^{2\pi} \int_0^{\pi} r\sin\theta\cos\phi \frac{\sin^2(n\pi r/a)}{2\pi a r^2} r^2 \sin\theta \; d\theta d\phi dr = 0$$

Since $\int_0^{2\pi} \cos\phi = 0$ and for $y = r\sin\theta\sin\phi$ we get that

$$\int_{-\infty}^{\infty} y|\psi(r)|^2 \; dV = \int_0^a \int_0^{2\pi} \int_0^{\pi} r\sin\theta\sin\phi \frac{\sin^2(n\pi r/a)}{2\pi a r^2} r^2 \sin\theta \; d\theta d\phi dr = 0$$

Again because $\int_0^{2\pi} \sin\phi = 0$.

Therefore the mean position of the particle is at the origin.

Now we compute the variance of its height above the center as follows

$$\begin{aligned}
\int_{-\infty}^{\infty} z^2|\psi(r)|^2 \; dV &= \int_0^a \int_0^{2\pi} \int_0^{\pi} r^2\cos^2\theta \frac{\sin^2(n\pi r/a)}{2\pi a r^2} r^2 \sin\theta \; d\theta d\phi dr \\
&= \frac{1}{2\pi a} \int_0^a \int_0^{2\pi} \int_0^{\pi} r^2 \sin^2(n\pi r/a) \cos^2\theta \sin\theta \; d\theta d\phi dr \\
&= \frac{2}{3a} \int_0^a r^2 \sin^2(n\pi r/a) \; dr \\
&= \frac{2}{3} \frac{a^2(4\pi^3 n^3 - 6\pi n)}{24\pi^3 n^3}
\end{aligned}$$

□