Further Quantum Mechanics

Problem Set 1

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The TDSE reads:

$$\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}\right)^2\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{1}$$

Consider the right-hand side of the equation, we have:

$$\begin{aligned}\left(-i\hbar\nabla - q\mathbf{A}\right)^2\psi &= \left(i\hbar\nabla + q\mathbf{A}\right)\left(i\hbar\nabla\psi + q\mathbf{A}\psi\right)\\ &= -\hbar^2\nabla^2\psi + i\hbar q\nabla\cdot(\mathbf{A}\psi) + i\hbar q\mathbf{A}\cdot\nabla\psi + q^2\mathbf{A}^2\psi\end{aligned} \tag{2}$$

so that the TDSE becomes:

$$\frac{1}{2m}\left[i\hbar\nabla^2\psi + q\psi(\nabla\cdot\mathbf{A}) + 2q\mathbf{A}\cdot\nabla\psi + \frac{q^2}{i\hbar}\mathbf{A}^2\psi\right] = \frac{\partial\psi}{\partial t} \tag{3}$$

On the other hand, consider the time derivative of the probability density $\rho = \psi^*\psi$, we have:

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \frac{\partial}{\partial t}\left(\psi^*\psi\right)\\ &= \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\end{aligned} \tag{4}$$

Combining the two results, we have:

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \frac{\psi^*}{2m}\left[i\hbar\nabla^2\psi + q\psi(\nabla\cdot\mathbf{A}) + 2q\mathbf{A}\cdot\nabla\psi + \frac{q^2}{i\hbar}\mathbf{A}^2\psi\right]\\ &\quad+ \frac{\psi}{2m}\left[-i\hbar\nabla^2\psi^* + q\psi^*(\nabla\cdot\mathbf{A}) + 2q\mathbf{A}\cdot\nabla\psi^* - \frac{q^2}{i\hbar}\mathbf{A}^2\psi^*\right]\\ &= \frac{1}{2m}\left[i\hbar\left(\psi^*\nabla^2\psi + \psi\nabla^2\psi^*\right) + 2q\left(\psi^*\psi\right)(\nabla\cdot\mathbf{A}) + 2q\mathbf{A}\cdot\nabla\left(\psi^*\psi\right)\right]\\ &= \frac{\hbar}{2im}\left(\psi^*\nabla^2\psi + \psi\nabla^2\psi^*\right) + \frac{q}{m}\left[\psi^*\psi(\nabla\cdot\mathbf{A}) + \mathbf{A}\cdot\nabla\left(\psi^*\psi\right)\right]\\ &= -\nabla\cdot\mathbf{j}\end{aligned} \tag{5}$$

where we identify the probability current density $\mathbf{j}$ as:

$$\mathbf{j} = \frac{\hbar}{2im}\left(\psi^* \nabla \psi - \psi \nabla \psi^*\right) - \frac{q}{m}\mathbf{A}\psi^*\psi \tag{6}$$

Consider the TISE for an energy eigenfunction ψ:

$$\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}\right)^2 \psi = E\psi \tag{7}$$

Given the trial function $\psi(x, y) = \exp[-(x^2 + y^2)/4l_B^2]$, we have:

$$\begin{aligned}
\left(-i\hbar\nabla - q\mathbf{A}\right)^2 \psi &= -\hbar^2\nabla^2\psi + i\hbar q\psi\left(\nabla \cdot \mathbf{A}\right) + 2i\hbar q\mathbf{A} \cdot \nabla\psi + q^2\mathbf{A}^2\psi \\
&= -\hbar^2 \frac{x^2 + y^2 - 4l_B^2}{4l_B^4}\psi + \frac{B^2(x^2 + y^2)}{4}\psi
\end{aligned} \tag{8}$$

where the middle two terms vanish.

We can then solve the TISE:

$$\frac{B^2 l_B^4 (x^2 + y^2) - \hbar^2(x^2 + y^2 - 4l_B^2)}{4l_B^4}\psi = E\psi \tag{9}$$

We require that the coefficient for x and y to be zero, so that:

$$l_B = \sqrt{\frac{\hbar}{B}} \tag{10}$$

and the energy eigenvalue is:

$$E = 4\hbar^2 l_B^2 = 4\frac{\hbar^3}{B} \tag{11}$$

Since the eigenfunction is real, only the second term in $\mathbf{j}$ contributes:

$$\mathbf{j} = -\frac{qB}{2m}\exp\left(-\frac{x^2 + y^2}{2l_B^2}\right)(-y, x, 0)^\intercal \tag{12}$$

which is in the same direction as the magnetic field $\mathbf{B}$.

This describes the ground state of a charged particle in a magnetic field, which follows a helix trajectory around $\mathbf{B}$. The direction of $\mathbf{j}$ confirms this.

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Consider the Hamiltonian:

$$\hat{H} = \hat{H}_0 + \epsilon\hat{V} = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} + \epsilon \begin{pmatrix} B_1 & B_2 \\ B_2 & 0 \end{pmatrix} \tag{13}$$

where the first term is a simple Hamiltonian and the second term is a perturbation.

If $A_1 \neq A_2$, the energy eigenvalues of the unperturbed system are non-degenerate. The first-order correction to the energy eigenvalues is:

$$E_n^{(1)} = \langle n|\hat{V}|n\rangle \tag{14}$$

where $|n\rangle$ are the energy eigenstates of $\hat{H}_0$ given by:

$$|1\rangle = (1,0)^\intercal \qquad |2\rangle = (0,1)^\intercal \tag{15}$$

Then the first-order corrections are:

$$\begin{aligned} E_1^{(1)} &= \langle 1|\hat{V}|1\rangle = B_1 \\ E_2^{(1)} &= \langle 2|\hat{V}|2\rangle = 0 \end{aligned} \tag{16}$$

If $A_1 = A_2$, the energy eigenvalues of the unperturbed system are degenerate. We can diagonalise $\hat{V}$ to find the perturbation matrix in the basis of the degenerate energy eigenstates:

$$\hat{V} \to \frac{1}{2}\begin{pmatrix} B_1 - \sqrt{B_1^2 + 4B_2^2} & 0 \\ 0 & B_1 + \sqrt{B_1^2 + 4B_2^2} \end{pmatrix} \tag{17}$$

so that the first-order corrections are:

$$\begin{aligned} E_1^{(1)} &= \frac{1}{2}\left(B_1 - \sqrt{B_1^2 + 4B_2^2}\right) \\ E_2^{(1)} &= \frac{1}{2}\left(B_1 + \sqrt{B_1^2 + 4B_2^2}\right) \end{aligned} \tag{18}$$

We can also find the energy eigenstates from the Hamiltonian directly:

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(a) We have the perturbed Hamiltonian:

$$\hat{H} = \hat{H}_0 + \epsilon\hat{V} = \frac{1}{2}m\omega^2\hat{x}^2 + \epsilon\hat{x}^2 \tag{19}$$

But the perturbed system is still a harmonic oscillator, so the energy eigenstates change exactly to:

$$E'_n = \hbar(\kappa\omega)^2\left(n + \frac{1}{2}\right) \tag{20}$$

where $\kappa = \sqrt{1 + 2\epsilon/m\omega^2}$.

We could expand κ in terms of ϵ to second order:

$$\kappa \approx 1 + \frac{\epsilon}{m\omega^2} - \frac{\epsilon^2}{2m^2\omega^4} \tag{21}$$

so that the change in energy eigenvalues in the ground state is:

$$\Delta E_0 = E'_0 - E_0 = \frac{1}{2}\hbar\omega\left(\frac{\epsilon}{m\omega^2} - \frac{\epsilon^2}{2m^2\omega^4}\right) \tag{22}$$

(b) Treating this as a perturbation problem, we have the ground state wave function of the unperturbed system:

$$\psi_0(x) = \langle x|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{23}$$

The first-order correction to the ground state energy is:

$$\begin{aligned} E_0^{(1)} &= \langle 0|\hat{V}|0\rangle \\ &= \int \langle 0|x\rangle\ \langle x|\hat{V}|0\rangle\ \mathrm{d}x \\ &= \int \psi_0 x^2 \psi_0\,\mathrm{d}x \\ &= \frac{\hbar}{2m\omega} \end{aligned} \tag{24}$$

which indeed agrees with the previous result up to first order.

(c) The first-order correction to the ground state is:

$$\left|0^{(1)}\right\rangle = \sum_{m\neq 0} \frac{\langle m|\hat{V}|0\rangle}{E_0 - E_m} |m\rangle \tag{25}$$

Let us focus on the matrix element $\langle m|\hat{V}|0\rangle$:

$$\begin{aligned}\langle m|\hat{V}|0\rangle &= \int \langle m|x\rangle \langle x|\hat{V}|0\rangle \,\mathrm{d}x \\ &= \int \psi_m x^2 \psi_0 \,\mathrm{d}x\end{aligned} \tag{26}$$

We know that the energy eigenfunctions of a harmonic oscillator are Hermite polynomials of order n, so this integral is non-zero only when $m = 2$:

$$\langle 2|\hat{V}|0\rangle = \int \psi_2 x^2 \psi_0 \,\mathrm{d}x = \frac{\hbar}{\sqrt{2}m\omega} \tag{27}$$

which gives us the first-order correction to the ground state:

$$\left|0^{(1)}\right\rangle = \frac{\langle 2|\hat{V}|0\rangle}{E_0 - E_2} |2\rangle = \frac{\hbar}{\sqrt{2}m\omega} \frac{1}{-2\hbar\omega} |2\rangle = -\frac{l^2}{\sqrt{2}\hbar\omega} |2\rangle \tag{28}$$

where $l = \sqrt{\hbar/2m\omega}$ is the characteristic length scale of the harmonic oscillator.

(d) The second-order correction to the ground state energy is:

$$E_0^{(2)} = \sum_{m\neq 0} \frac{\langle 0|\hat{V}|m\rangle \langle m|\hat{V}|0\rangle}{E_0 - E_m} \tag{29}$$

Again, this sum is non-zero only when $m = 2$:

$$E_0^{(2)} = \frac{\langle 0|\hat{V}|2\rangle \langle 2|\hat{V}|0\rangle}{E_0 - E_2} = -\frac{\hbar}{4m^2\omega^3} \tag{30}$$

which also agrees with the previous result up to second order.

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