

Quantum Mechanics

Problem Sheet 2

Time Dependence, Schrödinger Equation & Wave Mechanics

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Time Dependence and the Schrödinger Equation

2.1

The time-dependent Schrödinger equation (TDSE) for the position wave function $\psi(x, t) \equiv \langle \hat{x} | \psi(t) \rangle$ is:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H} \psi(x, t) \quad (1)$$

while the time-independent Schrödinger equation (TISE) for the energy eigenfunction $\psi_n(x)$ is:

$$\hat{H} \psi_n(x) = E_n \psi_n(x) \quad (2)$$

Any wave function $\psi(x, t)$ must satisfy the TDSE but not necessarily the TISE. A wave function that satisfies the TISE is called an energy eigenfunction that only undergoes a phase change under time evolution.

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2.2

2.3

(a)

$$P(E \leq 6\varepsilon, t = 0) = \sum_{n=1,2} P(E = n^2\varepsilon, t = 0) = 0.2^2 + 0.3^2 = 0.13 \quad (3)$$

(b)

$$\begin{aligned} \langle E \rangle &= \sum E_n P(E = n^2\varepsilon, t = 0) \\ &= (1^2 \times 0.2^2 + 2^2 \times 0.3^2 + 3^2 \times 0.4^2 + 4^2 \times 0.843^2) \varepsilon \\ &= 13.210\varepsilon \end{aligned} \quad (4)$$

$$\begin{aligned} \langle E^2 \rangle &= \sum E_n^2 P(E = n^2\varepsilon, t = 0) \\ &= (1^4 \times 0.2^2 + 2^4 \times 0.3^2 + 3^4 \times 0.4^2 + 4^4 \times 0.843^2) \varepsilon^2 \\ &= 196.366\varepsilon^2 \end{aligned} \quad (5)$$

so that the rms deviation is:

$$\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2} = 4.675\varepsilon \quad (6)$$

(c) The time evolution of $|\psi(0)\rangle$ is given by:

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = \sum_n e^{-iE_n t/\hbar} c_n |n\rangle \quad (7)$$

so that after a time t , the probability of finding the system in the state $|j\rangle$ is:

$$P(j, t) = |\langle j | \psi(t) \rangle|^2 = \left| \sum_n e^{-iE_n t/\hbar} c_n \langle j | n \rangle \right|^2 = |c_j|^2 \quad (8)$$

which is unchanged because the time-evolution operator only changes the phase of each coefficient c_n .

Thus, the previous results still hold for $t > 0$.

(d) If energy is measured to be 16ε , then the system has ‘collapsed’ to the state $|\psi\rangle = |4\rangle$. We would only obtain the energy 16ε in any subsequent measurement of energy.

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2.4

Since the Hamiltonian \hat{H} and momentum operator \hat{p} commute, they share a common set of eigenfunctions and it is possible for a particle to have both well-defined energy and momentum. However, \hat{H} and position operator \hat{x} generally do not commute, so that a particle cannot have both well-defined energy and position.

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2.5

$$\begin{aligned} \langle \hat{x} \rangle &= \int_{-\infty}^{\infty} \psi^*(x, t) x \psi(x, t) dx \\ \langle \hat{x}^2 \rangle &= \int_{-\infty}^{\infty} \psi^*(x, t) x^2 \psi(x, t) dx \\ \langle \hat{p}_x \rangle &= \int_{-\infty}^{\infty} \psi^*(x, t) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x, t) dx \\ \langle \hat{p}_x^2 \rangle &= \int_{-\infty}^{\infty} \psi^*(x, t) \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi(x, t) dx \\ \langle \hat{H} \rangle &= \int_{-\infty}^{\infty} \psi^*(x, t) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) \psi(x, t) dx \end{aligned} \quad (9)$$

where the expectation for energy is given by the equation with the Hamiltonian operator \hat{H} .

The probability of finding the particle in (x_1, x_2) is:

$$P(x_1 < x < x_2) = \int_{x_1}^{x_2} |\psi(x, t)|^2 dx \quad (10)$$

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2.6

Any state $|\psi(t)\rangle$ must satisfy the TDSE:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (11)$$

and its bra counterpart:

$$-i\hbar \frac{\partial}{\partial t} \langle \psi(t)| = \langle \psi(t)| \hat{H} \quad (12)$$

We also know that $\hat{Q} |\psi(t)\rangle$, being a state itself, satisfies the TDSE:

$$i\hbar \frac{\partial}{\partial t} (\hat{Q} |\psi(t)\rangle) = \hat{H} \hat{Q} |\psi(t)\rangle \quad (13)$$

Assuming that \hat{Q} is a time-independent operator, consider the time derivative of its expectation:

$$\begin{aligned} \frac{d}{dt} \langle \hat{Q} \rangle &= \frac{d}{dt} (\langle \psi(t) | \hat{Q} | \psi(t) \rangle) \\ &= \left\langle \frac{\partial \psi}{\partial t} \right| \hat{Q} | \psi \rangle + \left\langle \psi \right| \hat{Q} \left| \frac{\partial \psi}{\partial t} \right\rangle \\ &= -\frac{1}{i\hbar} \langle \psi | \hat{H} \hat{Q} | \psi \rangle + \frac{1}{i\hbar} \langle \psi | \hat{Q} \hat{H} | \psi \rangle \\ &= \frac{1}{i\hbar} \langle \psi | [\hat{Q}, \hat{H}] | \psi \rangle \end{aligned} \quad (14)$$

which immediately gives the desired result.

Now let $\hat{Q} = \hat{x}$ and $[\hat{x}, \hat{H}]$ would be non-zero, so that the expectation of position is not conserved, i.e. constant in time. However, if $\hat{Q} = \hat{p}$, then $[\hat{p}, \hat{H}] = 0$ and the expectation of momentum is conserved.

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Wave Mechanics

2.7

In the region $x < 0$ and $V = 0$, the TISE is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad (15)$$

with the solution:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (16)$$

where $k \equiv \sqrt{2mE}/\hbar$.

In the region $0 < x$ and $V = V_0 < E$, the TISE is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi = E\psi \quad (17)$$

with the solution:

$$\psi(x) = Ce^{iKx} + De^{-iKx} \quad (18)$$

where $K \equiv \sqrt{2m(E - V_0)}/\hbar$.

The condition of no particle incident from $+\infty$ is $D = 0$.

Continuity of $\psi(x)$ and $\psi'(x)$ at $x = 0$ gives:

$$\begin{aligned} A + B &= C \\ ik(A - B) &= iKC \end{aligned} \quad (19)$$

solving which yields $B = A(k - K)/(k + K)$ and $C = 2Ak/(k + K)$.

Hence, the probability of reflection is the probability of finding the particle travelling to $-\infty$ in the region $x < 0$:

$$\left| \frac{B^2}{A^2} \right| = \left(\frac{k - K}{k + K} \right)^2 \quad (20)$$

Probability of transmission is:

$$\left| \frac{C^2}{A^2} \right| = \frac{4kK}{(k+K)^2} \quad (21)$$

The probability current on the left is:

$$\frac{i\hbar}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right) = \frac{\hbar}{m} \frac{kK}{k+K} = \frac{\hbar}{2m} \left(\frac{k-K}{k+K} \right) \quad (22)$$

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2.8

For bound states, we have $E < V_0$. Outside the well, the solution is:

$$\psi(x) = \begin{cases} De^{\kappa x} + D'e^{-\kappa x} & x < -a \\ Ce^{-\kappa x} + C'e^{\kappa x} & x > a \end{cases} \quad (23)$$

where $\kappa \equiv \sqrt{2m(V_0 - E)}/\hbar$.

and inside the well, the solution is:

$$\psi(x) = A \cos(kx) + B \sin(kx) \quad (24)$$

where $k \equiv \sqrt{2mE}/\hbar$.

For odd-parity solutions, we set $A = 0$ and $C = -D$ so that $\psi(x) = -\psi(-x)$. For the wave function to be finite, we also need $C' = D' = 0$. Continuity of $\psi(x)$ and $\psi'(x)$ at $x = \pm a$ gives:

$$\begin{aligned} B \sin(ka) &= Ce^{-\kappa a} \\ kB \cos(ka) &= -KCe^{-\kappa a} \\ -B \sin(ka) &= De^{-\kappa a} = -Ce^{-\kappa a} \\ kB \cos(ka) &= KDe^{-\kappa a} = -KCe^{-\kappa a} \end{aligned} \quad (25)$$

These can be solved to give:

$$\cot(ka) = -\frac{\kappa}{k} = -\sqrt{\frac{V_0}{E}} - 1 = -\sqrt{\frac{W^2}{(ka)^2} - 1} \quad (26)$$

where $W \equiv \sqrt{2mV_0a^2}/\hbar$.

For the square root to be valid, we must have $W > ka$ or $V_0 > E$. But for the cotangent to negative, we must have $ka > \pi/2$. Hence, we require $W > \pi/2$.

2.9

Consider the potential well:

$$V(x) = \begin{cases} -V_0 & |x| < a \\ 0 & \text{otherwise} \end{cases} \quad (27)$$

The solutions are:

$$\psi(x) = \begin{cases} De^{ikx} + re^{-ikx} & x < -a \\ Ae^{iKx} + Be^{-iKx} & -a < x < a \\ Ce^{-ikx} + te^{ikx} & x > a \end{cases} \quad (28)$$

where $k \equiv \sqrt{2mE}/\hbar$ and $K \equiv \sqrt{2m(V_0 + E)}/\hbar$.

Let us set $D = 1$ and $C = 0$ so that there is no particle incident from $+\infty$. Continuity of $\psi(x)$ and $\psi'(x)$ at $x = \pm a$ gives:

$$\begin{aligned} e^{-ika} + re^{ika} &= Ae^{-iKa} + Be^{iKa} \\ ik(e^{-ika} - re^{ika}) &= iK(Ae^{-iKa} - Be^{iKa}) \\ te^{ika} &= Ae^{iKa} + Be^{-iKa} \\ ikte^{ika} &= iK(Ae^{iKa} - Be^{-iKa}) \end{aligned} \quad (29)$$

These can be solved to give an expression for r :

$$r = \frac{e^{-2ika} (e^{4iKa} - 1) (k - K)(k + K)}{k^2 (e^{4iKa} - 1) - 2kK (1 + e^{4iKa}) + K^2 (e^{4iKa} - 1)} \quad (30)$$

Due to the factor $(e^{4iKa} - 1)$, $r = 0$ whenever $Ka = n\pi/2$ for $n \in \mathbb{Z}$. In this case, the particle is completely transmitted through the well and there is zero probability of observing a reflected particle.

2.10

Given the potential $V(x) = V_\delta \delta(x)$, the solutions are:

$$\psi(x) = \begin{cases} Ae^{ikx} + re^{-ikx} & x < 0 \\ Be^{-ikx} + te^{ikx} & x > 0 \end{cases} \quad (31)$$

where $k \equiv \sqrt{2mE}/\hbar$.

Again, let $B = 0$ so that there is no particle incident from $+\infty$. Continuity of $\psi(x)$ at $x = 0$ gives $A + r = t$. The continuity condition on $\psi'(x)$ is obtained by integrating the TISE around $x = 0$:

$$\begin{aligned} 0 &= \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \left[-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_\delta \delta(x)\psi - E\psi \right] dx \\ &= -\frac{\hbar^2}{2m} [\psi'(0^+) - \psi'(0^-)] + V_\delta \psi(0) \end{aligned} \quad (32)$$

which means:

$$ik(A - r + t) = K(A + r) \quad (33)$$

where $K \equiv \sqrt{2m(V_\delta + E)}/\hbar$.

Solving the equations yields $t = 2iAk/(2ik + K)$ and the probability of transmission is:

$$P_{\text{tun}} = \left| \frac{t}{A} \right|^2 = \left| \frac{1}{1 + K/2ik} \right|^2 = \frac{1}{1 + (K/2k)^2} \quad (34)$$

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2.11

Given the definition of the probability current density:

$$\mathbf{J}(\mathbf{r}, t) = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \quad (35)$$

we evaluate:

$$\begin{aligned} \psi &= Ae^{i(kz - \omega t)} + Be^{-i(kz - \omega t)} \\ \psi^* &= A^* e^{-i(kz - \omega t)} + B^* e^{i(kz - \omega t)} \\ \nabla \psi &= ik [Ae^{i(kz - \omega t)} - Be^{-i(kz - \omega t)}] \hat{z} \\ \nabla \psi^* &= -ik [A^* e^{-i(kz - \omega t)} - B^* e^{i(kz - \omega t)}] \hat{z} \end{aligned} \quad (36)$$

so that:

$$\begin{aligned}\mathbf{J}(\mathbf{r}, t) &= \hat{z} \frac{-\hbar k}{2m} (-2|A|^2 + 2|B|^2) \\ &= \frac{\hbar k}{m} (|A|^2 - |B|^2) \hat{z}\end{aligned}\quad (37)$$

The probability is proportional to the speed of the wave packet, and the minus sign is due to opposite directions of the wave packets.

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2.12

A momentum eigenstate, expressed in its position representation, is:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad (38)$$

with its complex conjugate:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \quad (39)$$

For a wave function of the form:

$$\psi(x, 0) = \langle x|\psi(0)\rangle = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} \exp\left(-\frac{x^2}{4\sigma^2} + \frac{ip_0x}{\hbar}\right) \quad (40)$$

its momentum representation is the integral:

$$\begin{aligned}\langle p|\psi(0)\rangle &= \int \langle p|x\rangle \langle x|\psi(0)\rangle dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} \int \exp\left[-\frac{x^2}{4\sigma^2} + \frac{i(p_0 - p)x}{\hbar}\right] dx\end{aligned}\quad (41)$$

Consider the change of variable:

$$y = \frac{x}{2\sigma} - \frac{i(p_0 - p)\sigma}{\hbar} \quad (42)$$

We have:

$$\begin{aligned}
\int \exp \left[-\frac{x^2}{4\sigma^2} + \frac{i(p_0 - p)x}{\hbar} \right] dx &= 2\sigma \int \exp \left[-y^2 - \left(\frac{p_0 - p}{\hbar} \right)^2 \sigma^2 \right] dy \\
&= \exp \left[-\frac{(p_0 - p)\sigma}{\hbar} \right]^2 2\sigma\sqrt{\pi}
\end{aligned} \tag{43}$$

so that the momentum representation is:

$$\langle p|\psi(0)\rangle = \left(\frac{2\sigma^2}{\pi\hbar^2} \right)^{1/4} \exp \left[-\frac{(p_0 - p)\sigma}{\hbar} \right]^2 \tag{44}$$

Note that $\langle p|\psi(0)\rangle$ just the Fourier transform of $\langle x|\psi(0)\rangle$:

$$\langle p|\psi(0)\rangle = \mathcal{F}[\langle x|\psi(0)\rangle] = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar} \langle x|\psi(0)\rangle dx \tag{45}$$

Consider a momentum eigenstate $|p\rangle$ that satisfies $\hat{p}|p\rangle = p|p\rangle$. Applying the Hamiltonian operator to $|p\rangle$ gives:

$$\hat{H}|p\rangle = \frac{\hat{p}^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle \tag{46}$$

which means that $|p\rangle$ is also an energy eigenstate with the eigenvalue $p^2/2m$.

The time-evolution of a momentum eigenstate $|p\rangle$ is hence given by:

$$|p\rangle \rightarrow e^{-i\hat{H}t/\hbar}|p\rangle = e^{-ip^2t/2m\hbar}|p\rangle \tag{47}$$

We may write $|\psi(0)\rangle$ as a superposition of momentum eigenstates so that its time-evolution is:

$$\begin{aligned}
|\psi(t)\rangle &= e^{-i\hat{H}t/\hbar}|\psi(0)\rangle \\
&= \int e^{-i\hat{H}t/\hbar}|p\rangle \langle p|\psi(0)\rangle dp \\
&= \int e^{-ip^2t/2m\hbar}|p\rangle \langle p|\psi(0)\rangle dp
\end{aligned} \tag{48}$$

Then the position representation of $|\psi(t)\rangle$ is:

$$\begin{aligned}
\psi(x, t) &= \langle x | \psi(t) \rangle \\
&= \int \exp\left(-\frac{ip^2t}{2m\hbar}\right) \langle x | p \rangle \langle p | \psi(0) \rangle dp \\
&= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/4} \int \exp\left[-\frac{ip^2t}{2m\hbar} + \frac{ipx}{\hbar} - \frac{(p_0 - p)^2\sigma^2}{\hbar^2}\right] dp \\
&= \left(\frac{2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2\sigma + i\hbar t/m\sigma}} \exp\left[-\frac{4mp_0\sigma^2x - 2p_0^2\sigma^2t + i\hbar mx^2}{-2\hbar^2t + 4i\hbar m\sigma^2}\right]
\end{aligned} \tag{49}$$

where the integral can be evaluated using a substitution similar to the previous one.

The square modulus of $\psi(x, t)$ is:

$$|\psi(x, t)|^2 = \frac{\sigma}{\sqrt{2\pi\hbar^2 |b(t)|^2}} \exp\left[-\frac{\sigma^2(x - p_0t/m)^2}{2\hbar^2 |b(t)|^2}\right] \tag{50}$$

where $b(t) \equiv \sigma^2/\hbar + it/2m$ and $|b(t)|^2 = \sigma^4/\hbar^2 + t^2/4m^2$.

As time goes on, the wave packet moves to the right and its variance/width increases:

$$\sigma^2(t) = \sigma^2 \left(1 + \frac{\hbar^2 t^2}{4m^2 \sigma^4}\right) \tag{51}$$

The particle gets ‘smeared out’ in space with an increasing uncertainty in its position due to an initial uncertainty in its momentum.

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