0.1 Preliminaries

$$
\begin{aligned}
\hbar &= 1.05 \times 10^{-34}\,\mathrm{J\,s} \\
\hbar c &= 297.3\,\mathrm{eV\,nm} \\
m_e &= 0.511\,\mathrm{MeV\,nm} \\
\frac{e^2}{4\pi\epsilon_0} &= 1.44\,\mathrm{eV\,nm} \\
\alpha = \frac{e^2/4\pi\epsilon_0}{\hbar c} &\sim \frac{1}{137} \\
hc &= 1240\,\mathrm{eV\,nm} \\
1\,\mathrm{u} &= 930\mathrm{MeV/c^2} \\
a_0 &= 0.05\,\mathrm{nm} = 0.5\,\text{Å} \\
1\,\mathrm{Ry} &= -13.6\,\mathrm{eV} \\
k_B T &= 0.025\,\mathrm{eV}(T \sim 290)
\end{aligned}
$$

0.1.1 Back of the envelope Calculation - Bohr radius and Rydberg energy

Find a_0 and $1\,\mathrm{Ry}$: $dpdx \sim \hbar \implies p \sim dp \sim \frac{\hbar}{a_0}$. Now minimizing the energy: $E = \frac{p^2}{2m_e} - \frac{e^2/4\pi\epsilon_0}{a_0} \sim \frac{\hbar^2}{2ma_0^2} - \frac{e^2/4\pi\epsilon_0}{a_0}$ gives E_{min} at $a_0 = \frac{\hbar^2}{me^2/4\pi\epsilon_0} = \frac{\hbar^2 c^2}{mc^2 \cdot e^2/4\pi\epsilon_0} = \frac{300^2}{0.511 \cdot 1.44} = 0.5\,\text{Å}$.

0.2 Introduction

Any square integrable function $\Psi(\mathbf{r}, t)$ describes a state of the system. It is called a probability density because the probability of finding a particle in a volume $\mathbf{r} \pm d^3r$ at a fixed time t is

$$
d^3r|\Psi(\mathbf{r}, t)|^2
$$

Moreover any superposition, that is a linear combination, also represents a state. Time evolution of a state is given by the Time-dependent Schrodinger equation. This equation is the «simplest» PDE that satisfies:

1. Einstein ($E = \hbar\omega$) and deBroglie ($p = \hbar/\omega$)
2. $E = \frac{p^2}{2m} + V(\mathbf{r}, t)$.
3. Linear in Ψ.

This gives $i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$.

0.2.1 Continuity Equation

Derivation gives: $\mathbf{J} = \frac{\hbar i}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)$,

$$
\frac{P(\mathbf{r}, t)}{t} + \operatorname{div}\mathbf{J} = 0
$$

$$
\begin{aligned}
\frac{d}{dt}\int d^3r P(\mathbf{r}, t) &= -\oint ds \mathbf{J} \cdot \hat{\mathbf{n}} \\
\mathbf{J} &= \frac{1}{2m}\left[\Psi^*\frac{\hbar}{i}\nabla\Psi + (\Psi^*\frac{\hbar}{i}\nabla\Psi)^*\right] \\
&= \frac{1}{m}\Re\left[\Psi^*\frac{\hbar}{i}\nabla\Psi\right]
\end{aligned}
$$

In the case of a plane wave, $\Psi = Ae^{i\left[\frac{\mathbf{pr}-E_p t}{\hbar}\right]}$ gives $\mathbf{J} = |A|^2\frac{\mathbf{p}}{m}$ (cf. fluid mechanics).

To show that $\hat{H}$ is hermitian:

$$0 = \frac{d}{dt}\int d^3r P(\mathbf{r},t) \qquad = \frac{d}{dt}\int d^3r - \operatorname{div} J$$

$$= \cdots$$

$$\int d^3r \Psi^*(H - H^*)\Psi$$

Since this works for all Ψ, $H - H^* = 0$ thus H^* is Hermitian. Note that in this class we *define* an operator A to be Hermitian if it satisfies:

$$\int d^3r \Psi^* \hat{A}\Psi == \int d^3r \Psi(\hat{A}\Psi)^*$$

0.3 Time independence

Assume that $V(\mathbf{r},t) = V(\mathbf{r})$ and $\Psi = \psi(\mathbf{r})\chi(t)$.

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$$
$$i\hbar\psi(\mathbf{r})\frac{d\chi}{dt} = [H\psi]\chi$$
$$i\hbar\frac{d\chi}{\chi} = \frac{1}{\psi}[H\psi]$$

The LHS is a function of time and the RHS is a function of $\mathbf{r}$. Therefore both are constant. Let E be this constant:

$$i\hbar\frac{d\chi}{\chi} = E \qquad H\Psi = E\Psi$$
$$\chi(t) = e^{-i(Et/\hbar)}$$
$$\therefore \Psi(\mathbf{r},t) = \psi(\mathbf{r})e^{-i(Et/\hbar)}$$

0.3.1 Free Particle

In the case of a free particle, $V \equiv 0$ and so by solving we will get in one dimension: $\Psi(x,t) = e^{i(px - \frac{p^2}{2m}t)/\hbar}$. Strange things happen:

1. Speed of a wave is given by the solution to the phase being constant. (Imagine sitting on top of a peak. In this frame, the phase at any given point does not move.) Therefore the speed of this particle is given by:

   $$px - \frac{p^2}{2m} \equiv \text{const} \implies \frac{dx}{dt} = \frac{p}{2m}$$

   which is half of the «expected» velocity.

2. Normalization of Ψ is not possible.

   One solution to this problem is to put the particle in a large box: $-L \leq x \leq L$, impose suitable boundary conditions and let $L \to \infty$ at the end of the calculation.[1]

   A more physical approach would be to treat $\Psi(x,t) = Ae^{i(px - \frac{p^2}{2m})/\hbar}$ as a tool so that we can decompose a state Ψ using a momentum eigenbasis:

   $$\Psi(x,t) = \int dp\, A_p e^{ipx/\hbar}e^{-iE_pt/\hbar}$$

[1] This will appear in solid state physics and condensed matter physics.

For convenience we can set $A_p = \frac{1}{\sqrt{2\pi\hbar}}\phi(p)$ to

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int dp\phi(p)e^{-i(px+E_pt)/\hbar}$$

0.3.2 Fourier Playground

Now, that we have two different descriptions of $\Psi(x,t)$: $\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int dp\phi(p)e^{-i(px+E_pt)/\hbar} = \psi(x)e^{-i(Et/\hbar)}$, we may use the fourier transform to swap between these two representations.

Theorem 0.1. [2] *If $f \in L^2$ (square integrable) and both f and f' are piecewise continuous then*

$$f(x) = \frac{1}{\sqrt{2\pi}}\int F(k)e^{ikx}dk$$

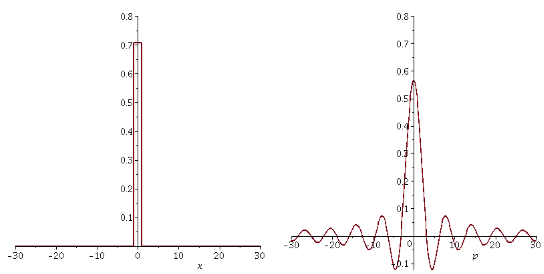
where

$$F(k) = \frac{1}{\sqrt{2\pi}}\int f(x)e^{-ikx}dx.$$

By setting $k = \frac{p}{\hbar}$ we get $f(x) \to \psi(x)$ and $F(k) \to \sqrt{\hbar}\phi(p)$.

Suppose we put a particle into a box, $-a < x < a$ with $\Psi(x,0) = \psi(x) = \begin{cases} \frac{1}{\sqrt{2a}} & -a < x < a \\ 0 & x \notin (-a,a) \end{cases}$. Then applying the FIT(0.1) we get:

$$\phi(p) = \frac{1}{\sqrt{2a}}\int \frac{e^{-ipx}}{\sqrt{2a}} = \frac{1}{\sqrt{\pi\hbar}}\frac{\sin(pa/\hbar)}{p/\hbar}$$



Note. This seemingly extreme behaviour above is due to the uncertainty principle. See wiki and appendix for more details. Someone mentioned in class that the different peaks of the position representation correspond to different energy levels; investigate.

Next, we wish to model a particle with a momentum of p_0. Therefore $e^{ip_0x/\hbar}$ has the largest contribution to $\Psi(x,t)$. Doing a first order expandsion of E_p:

$$E_p = E_0 + \left(\frac{dE}{dp}\right)_{p_0}(p - p_0) \equiv E_0 + E_0'(p - p_0)$$

Therefore

$$\begin{aligned}\Psi(x,t) &\sim \frac{1}{\sqrt{2\pi\hbar}}\int dp\phi(p)e^{i(px-E_0t)/\hbar}e^{iE_0'(p-p_0)t/\hbar} \\ &= e^{-i(E_0-E_0'p_0)t/\hbar}\int \frac{dp}{\sqrt{2\pi\hbar}}\phi(p)e^{ip(x-E_0't)/\hbar} \\ &= e^{-i(E_0-E_0'p_0)t/\hbar}\psi(x - E_0't)\end{aligned}$$

[2]In classical wave mechanics k denotes the wave number. Need an appendix on the Fourier transform. Consult wikipedia at: `http://en.wikipedia.org/wiki/Fourier_transform` and `http://en.wikipedia.org/wiki/Uncertainty_principle`

Therefore the wave packet seems to be moving with group velocity $v_g = E_0'$.

A first order approximation is good if and only if the second order error is small: $\Delta E_2 = \frac{1}{2}\left(\frac{d^2E}{dp^2}\right)_{p_0}(p-p_0)^2 = \frac{(\Delta p)^2}{2m}$. It turns out[3] that ΔE_2 represents the spread of the wave function and so there is negligible spread if:

$$\frac{\Delta E_2}{\hbar}t \ll 1 \implies \frac{(\Delta p)^2 t}{2m\hbar} \ll 1 \implies \frac{\hbar t}{2m(\Delta x)^2} \ll 1$$

Let D be the dimension of the apparatus in an experiment so that: $t \sim \frac{D}{v_g} = \frac{mD}{p_0}$ and $\frac{\hbar t}{2m(\Delta x)^2} \ll 1$ gives:

$$\frac{\hbar D}{2(\Delta x)^2 p_0} \ll 1 \implies \frac{\lambda_0 D}{4\pi(\Delta x)^2} \ll 1 \implies \frac{\Delta x}{\lambda_0} \gg \frac{D}{4\pi\Delta x}$$

Estimate: $D \sim 1\,\mathrm{mm}, \Delta x \sim 1\,\mathrm{nm} \implies \frac{D}{\Delta x} \gg 1$. Now magic[4]: thus the wave packet has negligible spread if $\Delta x/\lambda_0 \gg 1$. Thus, the wave packet must contain many deBroglie wavelengths.

0.4 Formal Theory

Statement of the 6 postulates. From P6, any measuremenet of a physical observable imply that the associated operator is Hermitian:

$$\int d^3r \Psi^* \hat{A}\Psi = \langle A\rangle = \langle A\rangle^* = \int d^3r \Psi(\hat{A}\Psi)^*$$

[3] Why?

[4] justify, I don't think this statement logically follow as it should