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Scattering States

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References

Wave mechanics and its applications, N. F. Mott and I. N. Sneddon, §I.3 (Chem QC174.1 M85).

Quantum Mechanics, L. I. Schiff, §17 (Chem QC174.1 S34 1955).

1 unit vol @ some pt in time

The probability flux

Sq The wavefunction = probability density

due to time evolution probability moves around

If the probability of finding an electron in a volume v at time t is

$$\int_v dr\, |\Psi(r,t)|^2,$$

$|\Psi(r,t)|^2$ is the *probability density*. As $\Psi(r,t)$ changes in time,

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \Psi(r,t) + V(r)\Psi(r,t),$$

the probability density changes in time and there is an associated *probability flux*

$$J(r,t) = -\frac{i\hbar}{2m}[\Psi^*(r,t)\nabla\Psi(r,t) - \Psi(r,t)\nabla\Psi^*(r,t)]. \tag{1}$$

If $\Psi(r,t) = e^{-iEt/\hbar}\psi(r)$,

$$J(r) = -\frac{i\hbar}{2m}[\psi^*(r)\nabla\psi(r) - \psi(r)\nabla\psi^*(r)]. \tag{2}$$

Bound *versus* unbound states

A *bound* state of energy E is a solution to

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r) \tag{3}$$

for which $\psi(r) \to 0$ as $|r| \to \infty$. For such states $\psi(r)$ can always be *normalized*, i.e., scaled so that

$$\int_{\textit{all space}} dr\, |\psi(r)|^2 = 1,$$

as a probability interpretation requires. If $\psi(\boldsymbol{r}) \not\to 0$ as $|\boldsymbol{r}| \to \infty$, $\psi(\boldsymbol{r})$ is an *unbound* state. Such states are called *scattering states* for there is an associated non-zero probability flux $\boldsymbol{J}$.

In one-dimension, the state

$$\psi(x) = Ce^{ikx}$$

has a well-defined momentum $p = \hbar k$ and thus represents a 'beam' of particles with velocity $\hbar k/m$. $|C|^2$ is the *density* of the particles in the beam, this interpretation replacing the probabilistic interpretation. A solution to (3) that looks like

$$\begin{cases} e^{i\ell x} + Ae^{-i\ell x} & , \text{as } x \to -\infty, \\ De^{i\ell x} & , \text{as } x \to +\infty, \end{cases}$$

is interpreted as representing a stationary scattering experiment: A beam of particles with velocity $\ell\hbar/m$ starts from the left and is reflected with probability $|A|^2$ or transmitted with probability $|D|^2$.

Problem Set #2

1. Bound states can be made real.

   Show that a bound state with $J(r) \equiv 0$ can always be taken as a *real* function. That is, identify how the phase of a state with $J(r) \equiv 0$ varies with r.

2. Scattering off a barrier.

   Consider scattering off the one-dimensional potential barrier

$$V(x) = \begin{cases} 0, & x < 0, \\ V, & 0 \le x \le L, \\ 0, & L < x, \end{cases} \tag{1}$$

with $V = 1$ and $L = 5$. If state functions are assumed to have the form

$$\psi(x) = \begin{cases} (1 + A) \cos kx + i(1 - A) \sin kx, & x < 0, \\ Be^{\ell x} + Ce^{-\ell x}, & 0 \le x \le L, \\ D(\cos kx + i \sin kx), & L < x, \end{cases} \tag{2}$$

calculate $|A|^2$, $|D|^2$ and $|A|^2 + |D|^2$.

> While *Mathematica* has Abs[ ] and ComplexConjugate[ ] functions, these are not useful with symbolic expressions because *Mathematica* doesn't know that the symbols (like k, ℓ and L) stand for real numbers. Thus $|A|^2$ must be calculated "by hand". While this can be done literally with paper and pencil, you might also succeed with this devious approach: First use J in place of the square root of minus one in the definitions of the wavefunction. [*Mathematica* won't know what J is, of course.] Then if you carry out the determination of A you will get an expression which has a J in it. Let 'aj' represent this expression. To find Abs[]^2, you can form (aj/.J–> I)*(aj/.J–> –I) and hope that Simplify[] will succeed in removing all the symbolic I's.

Note that (2) gives the correct form for $f(x)$ in $0 \le x \le L$ **only if** $0 \le E \le 1$. Another representation will have to be used when $E > 1$.

Make a plot of the transmission probability as a function of E for $0 \le E \le 3$. Make a similar plot for the reflection probability. Turn in a single plot that shows both these curves.

3. Scattering off a well.

Consider scattering off the potential well (considered in Problem Set #1)

$$V(x) = \begin{cases} V, & x < 0, \\ 0, & 0 \le x \le L, \\ V, & L < x, \end{cases}$$

with $V = 1$ and $L = 5; .5$. If state functions are assumed to have the form

$$\psi(r) = \begin{cases} (1+A)\cos \ell x + i(1-A)\sin \ell x, & x < 0, \\ (B+C)\cos kx + i(B-C)\sin kx, & 0 \le x \le L, \\ D[\cos \ell(x-L) + i \sin \ell(x-L)], & L < x, \end{cases}$$

calculate $|A|^2$, $|D|^2$ and $|A|^2 + |D|^2$.

In this case the energy of the incident electron must be ≥ 1. Plot the transmission probability $T(E)$ as a function of E for $1 \le E \le 7$. Identify the first 3 energies at which the transmission probability is 1. For scattering with these energies, what is the ratio of the value of $|\psi(x)|^2$ inside the well to the value outside the well?