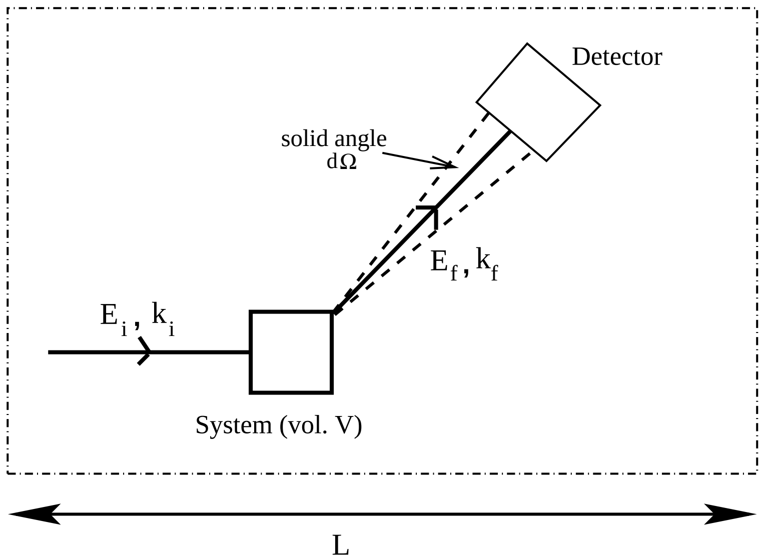
Physics 219
Van Hove Scattering Formula[1]

Consider a scattering experiment in which a particle of mass m, wavevector $\mathbf{k}_i$, and energy E_i is incident on a system, after which it is scattered to a state with energy E_f and wavevector within a solid angle $d\Omega$ about $\mathbf{k}_f$.



We define

$$\mathbf{k}_f - \mathbf{k}_i = \hbar\mathbf{q}\,, \tag{1}$$
$$E_f - E_i = \hbar\omega\,, \tag{2}$$

so $\hbar\omega$ is the energy *gained* by the system and $\hbar\mathbf{q}$ is the momentum *imparted* to the system. The objective is to calculate the partial differential scattering cross section $d^2\sigma/d\Omega dE_f$. This is defined as follows:

> $(d\Omega dE_f)\ d^2\sigma/d\Omega dE_f$ is the number of particles scattered per unit time into solid angle $d\Omega$ about $\mathbf{k}_f$ with an energy within dE_f about E_f, divided by the incident flux.

The flux is the number of particles crossing unit area per unit time.

To do the calculation it is convenient to normalize the wavefunction of the particles in a large box of size L^3. Since the box is artificial (but convenient) its size must drop out of the final answer (which it does). The wave functions of the particle then have the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{L^{3/2}} \exp(i\mathbf{k}\cdot\mathbf{r})\,. \tag{3}$$

We assume that the particle interacts quite weakly with the system and we use the Born approximation (which comes from leading order time-dependent perturbation theory) to calculate the cross section. This assumption is quite good for neutrons which are electrically neutral, but not satisfactory for electrons, which interact strongly because they are electrically charged.

If the particle is at $\mathbf{r}$, then its interaction with the system is written as

$$\int d^3r' \, A(\mathbf{r}') u(\mathbf{r}' - \mathbf{r}) \,, \tag{4}$$

where $A(\mathbf{r})$ is the "density" of the system with which the probe interacts, and $u(\mathbf{r})$ is the potential energy of interaction. For example, neutrons interact with the nuclei of the system through the contact interaction

$$\frac{2\pi\hbar^2}{2m} \, b \sum_l \delta(\mathbf{r} - \mathbf{R}_l) \tag{5}$$

where $\mathbf{R}_l$ is the position of the l-th nucleus of the system, and b is called the scattering length. This corresponds to Eq. (4) with

$$A(\mathbf{r}) \;=\; \sum_l \delta(\mathbf{r} - \mathbf{R}_l), \qquad \text{(the nuclear density)} \tag{6}$$

$$u(\mathbf{r} - \mathbf{r}') \;=\; \frac{2\pi\hbar^2}{2m} \, b \; \delta(\mathbf{r} - \mathbf{r}') \,. \tag{7}$$

We will need to the Fourier transform of the interaction

$$U(\mathbf{q}) = \int d^3r \, u(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \,. \tag{8}$$

For example, for scattering of neutrons off nuclei we have

$$A(\mathbf{r}) \;=\; \sum_l e^{-i\mathbf{q}\cdot\mathbf{R}_l}, \tag{9}$$

$$U(\mathbf{q}) \;=\; \frac{2\pi\hbar^2}{2m} \, b, \quad \text{(independent of } \; \mathbf{q}). \tag{10}$$

In the **Born approximation**, the partial differential scattering cross section is given by

$$\boxed{\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} \left(\frac{m}{2\pi\hbar^2} \right)^2 |U(\mathbf{q})|^2 \sum_n P_n \sum_m |\langle n|A(\mathbf{q})|m\rangle|^2 \; \delta(E_n - E_m + \hbar\omega) \,,} \tag{11}$$

where $|n\rangle$ denotes an exact eigenstate of the system with energy E_n, and P_n is the Boltzmann probability for state $|n\rangle$. (We shall derive the Born approximation in class.)

It is most instructive to write Eq, (11) in another way. To do this we use the integral representation of the delta function

$$\delta(E_n - E_m + \hbar\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \, e^{i(E_n - E_m + \hbar\omega)/\hbar} \,. \tag{12}$$

We can therefore write

$$\langle n|A(\mathbf{q})|m\rangle \, e^{i(E_n - E_m)/\hbar} = \langle n|A(\mathbf{q}, t)|m\rangle, \tag{13}$$

where

$$A(\mathbf{q}, t) = e^{i\mathcal{H}t/\hbar} \, A(\mathbf{q}) \, e^{-i\mathcal{H}t/\hbar} \tag{14}$$

is the time-dependent operator in the Heisenberg picture, and $\mathcal{H}$ is the Hamiltonian of the system. We can now use the closure rule

$$\sum_m |m\rangle \langle m| = 1, \tag{15}$$

and denote statistical mechanics averages $\sum_n P_n \langle n| \cdots |n\rangle$ by $\langle \cdots \rangle$, and thereby obtain the **van Hove scattering formula**

$$\boxed{\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} \left(\frac{m}{2\pi\hbar}\right)^2 \frac{|U(\mathbf{q})|^2}{2\pi\hbar} \int_{-\infty}^{\infty} dt \, \langle A(\mathbf{q},t) A(-\mathbf{q},0)\rangle \, e^{i\omega t} \, .} \tag{16}$$

This shows that the cross section depends on space and time dependent correlations in the system.

Let us separate out the part of Eq. (16) which involves the coordinates of the system and write

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} \left(\frac{m}{2\pi\hbar}\right)^2 \frac{|U(\mathbf{q})|^2}{2\pi\hbar} V \, S(\mathbf{q},\omega) \, , \tag{17}$$

where

$$\begin{aligned} S(\mathbf{q},\omega) &= \boxed{\frac{1}{V} \int_{-\infty}^{\infty} dt \, \langle A(q,t) A(-q,0)\rangle \, e^{i\omega t}} \\ &= \frac{1}{V} \int_{-\infty}^{\infty} dt \int d^3r_1 d^3r_2 \, \langle A(\mathbf{r}_1,t) A(\mathbf{r}_2,0)\rangle \, e^{i\omega t - \mathbf{q}\cdot(\mathbf{r}_1 - \mathbf{r}_2)} \, , \end{aligned} \tag{18}$$

is called the **dynamical structure factor**. In the time domain, $\langle A(\mathbf{r}_1,t) A(\mathbf{r}_2,0)\rangle$ is called a **correlation function**. In many situations we have translational invariance, so $\langle A(\mathbf{r}_1,t) A(\mathbf{r}_2,0)\rangle$ only depends on $\mathbf{r}_1 - \mathbf{r}_2$, in which case

$$\boxed{S(\mathbf{q},\omega) = \int_{-\infty}^{\infty} dt \int d^3r \, \langle A(\mathbf{r},t) A(0,0)\rangle \, e^{i\omega t - \mathbf{q}\cdot\mathbf{r}}} \, . \tag{19}$$

We have obtained the important result that scattering experiments give direct information on space and time-dependent correlations in the system.

In the next lecture we will discuss linear response theory, the response of the system to an external perturbation which is assumed small. We shall see that the resulting "linear response function" is also related to the space and time dependent correlations of the system, the most direct connection being the "fluctuation-dissipation theorem". It is therefore important to be able to calculate linear response functions and the related correlation functions using statistical mechanics.

The most detailed and systematic approach for such calculations, using diagrammatic perturbation theory techniques borrowed from field theory, is called "many body theory" and is outside the scope of this course. In the last lecture of the class, we shall briefly discuss another approach to calculating linear response functions, which is simpler but less systematic, known as the equations of motion method.

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[1] W. Marshall and S. W. Lovesey "*Theory of Thermal Neutron Scattering*", Oxford University Press.