

## Supplement 2.A

### 2.2.1 Green's function

The solution of the Schrödinger equation for  $E > 0$  (*scattering states*) is denoted by  $\psi_{\mathbf{k}}^+(r)$  where the plus sign indicates that the asymptotic behavior is that of an outgoing spherical wave.  $\psi_{\mathbf{k}}^-(r)$  is also a solution of the same Schrödinger equation but has the asymptotic behavior of an incoming spherical wave. From time-reversal invariance

$$\psi_{\mathbf{k}}^{-*}(\mathbf{r}) = \psi_{-\mathbf{k}}^+(\mathbf{r}), \quad (2.22)$$

which gives, from Eq. 2.8,

$$\psi_{\mathbf{k}}^-(\mathbf{r}) \xrightarrow{r \rightarrow \infty} e^{i\mathbf{k} \cdot \mathbf{r}} + f^*(\pi - \theta) \frac{e^{-ikr}}{r}. \quad (2.23)$$

Thus, we concentrate on  $\psi_{\mathbf{k}}^+$  and if the sign is not given  $\psi_{\mathbf{k}}^+$  is understood. We denote  $\phi_{\mathbf{k}} = e^{i\mathbf{k} \cdot \mathbf{r}}$ .

The Schrödinger equation is

$$(E - H_0)\psi_{\mathbf{k}}(\mathbf{r}) = V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}), \quad (2.24)$$

where  $H_0$  is the kinetic energy operator.  $\phi_{\mathbf{k}}$  obeys the equation

$$(E - H_0)\phi_{\mathbf{k}} = 0. \quad (2.25)$$

It also obeys the equation

$$(E - H_0)\phi_{\mathbf{k}'} = (E - E')\phi_{\mathbf{k}'}, \quad (2.26)$$

the orthogonality condition

$$\int \phi_{\mathbf{k}}^*(\mathbf{r}')\phi_{\mathbf{k}'}(\mathbf{r})d^3r = (2\pi)^3\delta(\mathbf{k} - \mathbf{k}'), \quad (2.27)$$

and the closure relation

$$\int \phi_{\mathbf{k}}^*(\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r})d^3k = (2\pi)^3\delta(\mathbf{r} - \mathbf{r}'). \quad (2.28)$$

It is useful to expand the scattering solution in terms of  $\phi_{\mathbf{k}}$ ,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \int a(\mathbf{k}')\phi_{\mathbf{k}'}(\mathbf{r})d^3k'. \quad (2.29)$$

Using this in Eq. 2.26, Eq. 2.24 becomes

$$\int a(\mathbf{k}')(E - E')\phi_{\mathbf{k}'}(\mathbf{r})d^3k' = V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}). \quad (2.30)$$

Multiplying by  $\phi_{\mathbf{k}}^*(\mathbf{r})$ , integrating over  $\mathbf{r}$ , and using 2.28 we get

$$(2\pi)^3(E - E')a(\mathbf{k}') = \int \phi_{\mathbf{k}'}^*(\mathbf{r})V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r})d^3r. \quad (2.31)$$

Putting this back into Eq. 2.29 we have

$$\psi_{\mathbf{k}}(\mathbf{r}) = \int a(\mathbf{k}')\phi_{\mathbf{k}'}(\mathbf{r})d^3k' = \int G_0(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d^3r' \quad (2.32)$$

where  $G_0(\mathbf{r}, \mathbf{r}')$  is given by

$$G_0(\mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi)^3} \int \frac{\phi_{\mathbf{k}'}(\mathbf{r})\phi_{\mathbf{k}'}^*(\mathbf{r}')}{E - E'}d^3k'. \quad (2.33)$$

The general solution of Eq. 2.24 is obtained by adding any solution of the homogeneous Eq. 2.25 to Eq. 2.32. I.e.,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int G_0(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d^3r'. \quad (2.34)$$

Using 2.26 we obtain that  $G_0(\mathbf{r}, \mathbf{r}')$  satisfies the equation

$$(E - H_0)G_0(\mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi)^3} \int e^{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')}d^3k = \delta(\mathbf{r} - \mathbf{r}'). \quad (2.35)$$

Eq. 2.33 has poles in  $k = \pm k'$ . We can eliminate these poles by defining  $G_0(\mathbf{r}, \mathbf{r}')$  as

$$G_0^\pm(\mathbf{r}, \mathbf{r}') = \lim_{\eta \rightarrow 0^\pm} \frac{1}{(2\pi)^3} \frac{2m}{\hbar^2} \int \frac{\phi_{\mathbf{k}'}(\mathbf{r})\phi_{\mathbf{k}'}^*(\mathbf{r}')}{k^2 - k'^2 \pm i\eta}d^3k' \quad (2.36)$$

where  $\eta$  is a small positive quantity which is allowed to go to zero after the integration is performed. The integral in 2.36 is easily obtained by the residue technique. One gets

$$G_0^\pm(\mathbf{r}, \mathbf{r}') = -\frac{m}{2\pi\hbar^2} \frac{e^{\pm ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}. \quad (2.37)$$

The  $\pm$  sign arises from the residues in the  $k'$ -plane at  $+\eta$  and  $-\eta$ , respectively. Assuming that  $V(\mathbf{r}')$  falls off rapidly with  $r'$  so that in the asymptotic region  $r \gg r'$ , we can approximate

$$\begin{aligned} |\mathbf{r} - \mathbf{r}'|^{-1} &\rightarrow \frac{1}{r} \\ \exp\{\pm ik|\mathbf{r} - \mathbf{r}'|\} &\rightarrow \exp\{\pm i(kr - \mathbf{k}' \cdot \mathbf{r}')\} \end{aligned} \quad (2.38)$$

where  $\mathbf{k}' = k\hat{\mathbf{r}}$ .

Using 2.37, 2.38, and 2.34 we get

$$\psi_{\mathbf{k}}^{\pm}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} e^{i\mathbf{k} \cdot \mathbf{r}} - \frac{m}{2\pi\hbar^2} \frac{e^{\pm ikr}}{r} \int e^{\mp i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi_{\mathbf{k}}^{\pm}(\mathbf{r}') d^3r'. \quad (2.39)$$

Thus the  $\pm$  sign in  $G_0^{\pm}$  is associated with the  $\pm$  sign of  $\psi_{\mathbf{k}}$ .

As a by-product we obtain for the scattering amplitude

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi_{\mathbf{k}}^{\pm} d^3r'. \quad (2.40)$$

Multiplying 2.26 by  $(E - H_0)^{-1}$  we get

$$\frac{1}{E - H_0} (E - H_0) \phi_{\mathbf{k}'}(\mathbf{r}) = (E - E') \frac{1}{E - H_0} \phi_{\mathbf{k}'}(\mathbf{r})$$

from which we obtain

$$\frac{1}{E - H_0} \phi_{\mathbf{k}'}(\mathbf{r}) = \frac{1}{E - E'} \phi_{\mathbf{k}'}(\mathbf{r}). \quad (2.41)$$

Thus,  $\phi_{\mathbf{k}'}$  are eigenfunctions of the operator  $(E - H_0)^{-1}$ , with eigenvalues  $1/(E - E')$  where  $E' > 0$  and  $E \neq E'$ . For  $E = E'$  the operator  $(E - H_0)^{-1}$  is not defined. Similarly, from Eq. 2.24 we obtain

$$\psi_{\mathbf{k}}(\mathbf{r}) = (E - H_0)^{-1} V(\mathbf{r}) \psi_{\mathbf{k}}(\mathbf{r}).$$

Removing the divergence by inserting a small quantity  $\eta$  and adding the solution of the homogeneous equation we get the formal solution

$$\psi_{\mathbf{k}}^{\pm}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + (E - H_0 \pm i\eta)^{-1} V(\mathbf{r}) \psi_{\mathbf{k}}(\mathbf{r}). \quad (2.42)$$

This is a solution of the Schrödinger equation only when  $\eta \rightarrow 0$ .

Comparing 2.34 with 2.42 we see that formally the Green's function is given by

$$G_0^{\pm} = \frac{1}{E - H_0 \pm i\eta}. \quad (2.43)$$

We can check this by using Eq. 2.41 which can be written in the more general form

$$\frac{1}{E - H + i\eta} |m\rangle = \frac{1}{E - E_m + i\eta} |m\rangle$$

where  $H$  is any Hamiltonian and  $|m\rangle$  are the corresponding eigenfunctions. Multiplying on the right by  $\langle m|$ , summing over  $m$  and using closure ( $\sum_m |m\rangle \langle m| = 1$ ) we get

$$\frac{1}{E - H + i\eta} = \sum_m \frac{1}{E - E_m + i\eta} |m\rangle \langle m| \quad (2.44)$$

where  $\sum_m$  implies summation over discrete eigenstates and integration over continuous eigenstates. If  $H$  is replaced by the kinetic energy operator  $H_0$  and  $|m\rangle$  are replaced by the continuous eigenstates  $(2\pi)^{-3/2} |\mathbf{k}\rangle$  equation 2.44 reduces to

$$\frac{1}{E - H_0 + i\eta} = \frac{1}{(2\pi)^3} \int d^3k' \frac{|\mathbf{k}'\rangle\langle\mathbf{k}'|}{E - E' + i\eta} \quad (2.45)$$

which is identical with Eq. 2.36,  $G_0(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r} | G_0 | \mathbf{r}' \rangle$ . Eq. 2.42 can also be written formally as

$$|\psi^\pm\rangle = |\phi\rangle + G_0^\pm V |\psi^\pm\rangle. \quad (2.46)$$

Eq. 2.46 is known as the *Lipmann-Schwinger equation*. It can be solved by iteration, first replacing  $|\psi^\pm\rangle$  by  $|\phi\rangle$  on its r.h.s., then replacing by  $|\phi\rangle + G_0^\pm V |\phi\rangle$ , and so on. This yields the *Lipmann-Schwinger series*.

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