Chapter 7

Propagators in one-particle quantum mechanics

In order to get used to the concept of a sp propagator in a many-particle system, it is useful to pose the problem for one particle using this language. In Sec. 7.1 the time evolution of a quantum state as generated by the Hamiltonian of the system is reviewed. The relation between a given initial state at an earlier time and the state at some later time suggests the definition of the propagator and relates it to the intuitive notion of Huygens' principle. The expansion of the propagator in terms of a known, or unperturbed, propagator is introduced in Sect 7.2 with special emphasis on its diagrammatic representation. A solution method for bound state problems is illustrated in Sec. 7.3, whereas a discussion of scattering using the propagator language is presented in Sec. 7.4.

7.1 Time evolution and propagators

Time evolution in physics is determined by the Hamiltonian of the physical system under study. In quantum mechanics one may denote the state of a particle with quantum numbers α at time t_0 by $|\alpha, t_0\rangle$. At time t one obtains the state $|\alpha, t_0; t\rangle$, which has evolved from the initial state, according to

$$|\alpha, t_0; t\rangle = e^{-\frac{i}{\hbar}H(t-t_0)}\,|\alpha, t_0\rangle \qquad t > t_0, \tag{7.1}$$

for a Hamiltonian that does not depend on time. The correctness of this result can be checked by inserting this expression in the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\,|\alpha, t_0; t\rangle = H\,|\alpha, t_0; t\rangle\,. \tag{7.2}$$

Equation (7.1) for $|\alpha, t_0; t\rangle$ can be written in terms of the wave function of the particle at time t as follows

$$\begin{aligned}\psi(\boldsymbol{r}, t) &= \langle \boldsymbol{r} | \alpha, t_0; t\rangle = \langle \boldsymbol{r}| e^{-\frac{i}{\hbar}H(t-t_0)} |\alpha, t_0\rangle \\ &= \int d^3r' \ \langle \boldsymbol{r}| e^{-\frac{i}{\hbar}H(t-t_0)} |\boldsymbol{r}'\rangle \langle \boldsymbol{r}'|\alpha, t_0\rangle \\ &= i\hbar \int d^3r' \ G(\boldsymbol{r}, \boldsymbol{r}'; t-t_0)\psi(\boldsymbol{r}', t_0) \qquad t > t_0, \quad (7.3)\end{aligned}$$

where G is referred to as the propagator or Green's function

$$G(\boldsymbol{r}, \boldsymbol{r}'; t-t_0) = -\frac{i}{\hbar} \langle \boldsymbol{r}| e^{-\frac{i}{\hbar}H(t-t_0)} |\boldsymbol{r}'\rangle . \qquad (7.4)$$

Its physical meaning can be illustrated by recalling Huygens' principle. Indeed, Eq. (7.3) illustrates that the wave function at $\boldsymbol{r}$ and t is determined by the wave function at the original time t_0, receiving contributions from all $\boldsymbol{r}'$ which are weighted by the amplitude G. Note that knowledge of the initial wave function and the propagator G thus allows the construction of the wavefunction at any time $t > t_0$.

Several alternative ways of writing the propagator may be obtained by using

$$H |n\rangle = \varepsilon_n |n\rangle \qquad (7.5)$$

for the exact eigenstates of H. By assuming a discrete spectrum for simplicity here, these alternative ways of writing the propagator include

$$\begin{aligned}G(\boldsymbol{r}, \boldsymbol{r}'; t-t_0) &= -\frac{i}{\hbar} \langle \boldsymbol{r}| e^{-\frac{i}{\hbar}H(t-t_0)} |\boldsymbol{r}'\rangle = -\frac{i}{\hbar} \langle 0| a_{\boldsymbol{r}} e^{-\frac{i}{\hbar}H(t-t_0)} a^\dagger_{\boldsymbol{r}'} |0\rangle \\ &= -\frac{i}{\hbar} \sum_n \langle 0| a_{\boldsymbol{r}} |n\rangle \langle n| a^\dagger_{\boldsymbol{r}'} |0\rangle e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)} \\ &= -\frac{i}{\hbar} \sum_n u_n(\boldsymbol{r}) u_n^*(\boldsymbol{r}') e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)} \qquad t > t_0. \quad (7.6)\end{aligned}$$

To include the causality condition $t > t_0$ explicitly, it is convenient to multiply the stepfunction $\theta(t-t_0)$ into this expression. For practical calculations it is essential to consider the Fourier transform (FT) of the propagator in order to arrive at useful nonperturbative (all order) solution methods. To work out this FT the following representation of the stepfunction can be used

$$\theta(t-t_0) = -\int \frac{dE'}{2\pi i} \ \frac{e^{-iE'(t-t_0)/\hbar}}{E' + i\eta}. \qquad (7.7)$$

Note that $\eta \downarrow 0$ is implied. For $t > t_0$, the integration path can be closed in the lower half plane and the contribution of the enclosed pole yields a result equal to 1. For $t < t_0$, one can close the contour in the upper half plane which yields a vanishing result since no pole is enclosed. At $t = t_0$ the stepfunction jumps from 0 to 1. As a result one obtains for the derivative

$$\frac{d}{dt}\theta(t-t_0) = \delta(t-t_0). \tag{7.8}$$

The FT of the propagator then reads in various alternative forms

$$\begin{aligned} G(\boldsymbol{r},\boldsymbol{r}';E) &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} d(t-t_0)\; e^{\frac{i}{\hbar}E(t-t_0)} \\ &\times \left\{\theta(t-t_0)\sum_n u_n(\boldsymbol{r})u_n^*(\boldsymbol{r}')e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}\right\} \\ &= \sum_n \frac{u_n(\boldsymbol{r})u_n^*(\boldsymbol{r}')}{E-\varepsilon_n+i\eta} = \sum_n \frac{\langle 0|\, a_{\boldsymbol{r}}\,|n\rangle\,\langle n|\, a_{\boldsymbol{r}'}^\dagger\,|0\rangle}{E-\varepsilon_n+i\eta} \\ &= \langle 0|\, a_{\boldsymbol{r}}\frac{1}{E-H+i\eta}a_{\boldsymbol{r}'}^\dagger\,|0\rangle = \langle \boldsymbol{r}|\,\frac{1}{E-H+i\eta}\,|\boldsymbol{r}'\rangle\,. \end{aligned} \tag{7.9}$$

The inclusion of the $i\eta$ term in the denominator therefore results from the inclusion of condition $t > t_0$ (time going forward). The formulation in Eq. (7.9) assume that a spinless boson is considered. The inclusion of spin quantum numbers makes the notation appropriate for a fermion but only complicates the notation. Some of the expressions for G will have their counterpart for the sp propagator in a many-particle system. It is important to realize that one can consider the propagator in any sp basis

$$G(\alpha,\beta;E) = \langle 0|\, a_\alpha \frac{1}{E-H+i\eta} a_\beta^\dagger\,|0\rangle\,, \tag{7.10}$$

where α represents an appropriate set of sp quantum numbers to identify a possible state of the particle.

7.2 Expansion of the propagator and diagram rules

The exact propagator can be related to an approximate propagator by using a decomposition of the Hamiltonian

$$H = H_0 + V, \tag{7.11}$$

where H_0 is referred to as the unperturbed Hamiltonian for which the corresponding propagator $G^{(0)}$ is readily available. The following operator identity

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A}B\frac{1}{A-B}, \tag{7.12}$$

with $A = E - H_0 + i\eta$ and $B = V$ may then be employed. This operator equation relates the operator for G, involving H,

$$G = \frac{1}{E - H + i\eta} \tag{7.13}$$

to the corresponding operator $G^{(0)}$, involving H_0, and the potential V

$$\begin{aligned} G &= G^{(0)} + G^{(0)}\ V\ G \\ &= G^{(0)} + G^{(0)}\ V\ G^{(0)} + G^{(0)}\ V\ G^{(0)}\ V\ G^{(0)} + ... \end{aligned} \tag{7.14}$$

The unperturbed propagator, which is given by

$$G^{(0)}(\alpha,\beta;E) = \langle 0|\, a_\alpha \frac{1}{E - H_0 + i\eta} a^\dagger_\beta\, |0\rangle\,, \tag{7.15}$$

can then be used to obtain

$$\begin{aligned} \langle\alpha|\,\frac{1}{E-H+i\eta}\,|\beta\rangle &= \langle\alpha|\,\frac{1}{E-H_0+i\eta}\,|\beta\rangle \\ &\quad + \sum_{\gamma\delta}\langle\alpha|\,\frac{1}{E-H_0+i\eta}\,|\gamma\rangle\,\langle\gamma|\,V\,|\delta\rangle\,\langle\delta|\,\frac{1}{E-H+i\eta}\,|\beta\rangle \end{aligned} \tag{7.16}$$

or

$$G(\alpha,\beta;E) = G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\,\langle\gamma|\,V\,|\delta\rangle\,G(\delta,\beta;E). \tag{7.17}$$

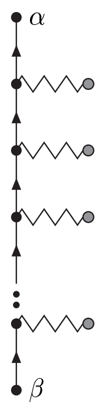
7.2.1 *Diagram Rules for the Single-Particle Propagator*

It is possible to generate a series of diagrams which represent the contributions to the sp propagator in a perturbation expansion in the potential V. These terms can be obtained algebraically by iterating the equation for the sp propagator. It is convenient to choose $\{|\alpha\rangle\}$ to be eigenstates of H_0 with eigenvalues $\{\varepsilon_\alpha\}$. One then obtains

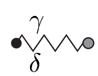
$$G^{(0)}(\alpha,\beta;E) = \frac{\delta_{\alpha,\beta}}{E - \varepsilon_\alpha + i\eta}. \tag{7.18}$$

For a contribution of k^{th} order in V one finds

Rule 1 Draw a directed line with k zigzag (horizontal) interaction lines V and $k+1$ directed unperturbed propagators $G^{(0)}$



Rule 2 Label external points (α and β)
Label each V



$\langle\gamma|\,V\,|\delta\rangle$

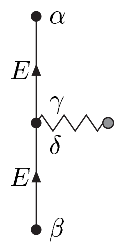
For each full line with arrow write

$G^{(0)}(\mu,\nu;E)$

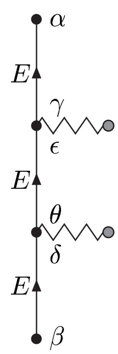
Rule 3 Sum (integrate) over all internal quantum numbers

Examples of diagrams in the single-particle problem

$G^{(0)}(\alpha,\beta;E)$



$$\sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\,\langle\gamma|\,V\,|\delta\rangle\,G^{(0)}(\delta,\beta;E)$$



$$\begin{aligned}&\sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\\ &\qquad\times\left\{\sum_{\epsilon\theta}\langle\gamma|\,V\,|\epsilon\rangle\,G^{(0)}(\epsilon,\theta;E)\,\langle\theta|\,V\,|\delta\rangle\right\}G^{(0)}(\delta,\beta;E)\end{aligned}$$

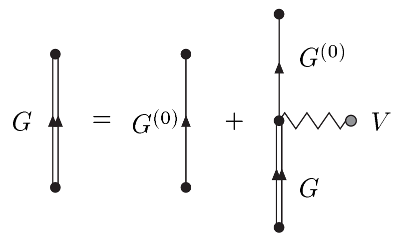
One can easily extend this to third and higher order terms in V. Similar diagrams will be generated when the sp propagator will be considered in a many-body system and it is useful to illustrate some of the possible resummations of the diagrams that can be considered. To avoid cluttering notation one may use the operator form (Eq. (7.14)) to rearrange the series corresponding to the sum of all diagrams in several ways

$$\begin{aligned}G &= G^{(0)} + G^{(0)}\ V\ G^{(0)} + G^{(0)}\ V\ G^{(0)}\ V\ G^{(0)} + ... \\ &= G^{(0)} + G^{(0)}\ V\ \{G^{(0)} + G^{(0)}\ V\ G^{(0)} + ...\} = G^{(0)} + G^{(0)}\ V\ G \\ &= G^{(0)} + \{G^{(0)} + G^{(0)}\ V\ G^{(0)} + ...\}\ V\ G^{(0)} = G^{(0)} + G\ V\ G^{(0)} \\ &= G^{(0)}\ + G^{(0)}\{V + V\ G^{(0)}\ V + ...\}\ G^{(0)} = G^{(0)} + G^{(0)}\ T\ G^{(0)},\end{aligned} \tag{7.19}$$

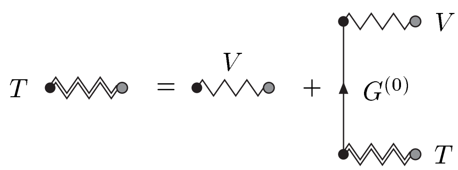
where

$$\begin{aligned}T &= V + V\ G^{(0)}\ V + V\ G^{(0)}\ V\ G^{(0)}\ V + ... \\ &= V + V\ G^{(0)}\ \left\{V + V\ G^{(0)}\ V + ...\right\} \\ &= V + V\ G^{(0)}\ T = V + T\ G^{(0)}\ V = V + V\ G\ V.\end{aligned} \tag{7.20}$$

A compact way to depict $G = G^{(0)} + G^{(0)} V G$ diagrammatically is given by:



The double line is used to represent G. Similar diagrammatic results can be obtained for the other forms of Eq. (7.19). T is simply the T-matrix used for the calculation of the scattering amplitude. The corresponding equations in Eq. (7.20 represent possible forms for the Lippmann-Schwinger equation. One may also use a diagrammatic representation of Eq. (7.20) as follows:



This formulation in terms of T-matrices, each diagrammatically represented by a double zigzag line, can be quite practical in the case of continuum solutions. Considering again the problem in which V represents a localized potential and $H_0 = T$, one can choose the sp basis $\{|\alpha\rangle = |\boldsymbol{p}\rangle\}$ to obtain

$$\langle \boldsymbol{p}_1 | \, T(E) \, | \boldsymbol{p}_2 \rangle = \tag{7.21}$$
$$\langle \boldsymbol{p}_1 | \, V \, | \boldsymbol{p}_2 \rangle + \int d\boldsymbol{p} \, \langle \boldsymbol{p}_1 | \, V \, | \boldsymbol{p} \rangle \, \frac{1}{E - p^2/2m + i\eta} \, \langle \boldsymbol{p} | \, T(E) \, | \boldsymbol{p}_2 \rangle$$

for a particle without spin.

7.3 Solution in the case of discrete states

A general procedure can now be used to obtain from the equation for G relevant information related to the possible discrete states of H. This procedure can also be used to solve the corresponding propagator equation in the medium with both an energy-independent as well as an energy-dependent potential. In the present case, familiar results will be obtained but it is useful to illustrate this procedure since it can be straightforwardly adapted in more complicated situations. One may denote the exact eigenkets and

-energies of H by

$$H\,|m\rangle = \varepsilon_m\,|m\rangle$$

for possible discrete states ($\varepsilon_m < 0$) and by

$$H\,|\mu\rangle = \varepsilon_\mu\,|\mu\rangle$$

for continuum states ($\varepsilon_\mu > 0$). Using the completeness relation for the exact eigenstates of H

$$1 = \sum_m |m\rangle\,\langle m| + \int d\mu\;\; |\mu\rangle\,\langle\mu| \tag{7.22}$$

one obtains for Eq. (7.10)

$$G(\alpha,\beta;E) = \sum_m \frac{\langle\alpha|m\rangle\langle m|\beta\rangle}{E-\varepsilon_m+i\eta} + \int d\mu\;\frac{\langle\alpha|\mu\rangle\langle\mu|\beta\rangle}{E-\varepsilon_\mu+i\eta}. \tag{7.23}$$

Proceeding with the assumption that $H_0 = T$ and V is an energy-independent, localized, but not necesarily local potential, like in the case of a Woods-Saxon potential discussed in Sec 3.3, one may choose $\{|\alpha\rangle\} = \{|\boldsymbol{p}\rangle\}$ representing the eigenstates of T. To obtain the equation for the bound state energies from the propagator equation, one can use the following practival recipe. Calculate :

$$\lim_{E\to\varepsilon_n}(E-\varepsilon_n)\big\{G = G^{(0)} + G^{(0)}\;V\;G\big\}. \tag{7.24}$$

The three limits for each of the terms in this equation that need to be considered will now be considered one at a time. The limit of the left-hand side of Eq. (7.24) yields

$$\begin{aligned}\lim_{E\to\varepsilon_n}(E-\varepsilon_n)\left\{\sum_m \frac{\langle\alpha|m\rangle\langle m|\beta\rangle}{E-\varepsilon_m+i\eta} + ...\right\} &= \langle\alpha|n\rangle\langle n|\beta\rangle \\ &\Rightarrow \langle\boldsymbol{p}|n\rangle\langle n|\boldsymbol{p}'\rangle. \end{aligned} \tag{7.25}$$

For the first term on the right side of Eq. (7.24) one obtains

$$\begin{aligned}\lim_{E\to\varepsilon_n}(E-\varepsilon_n)\,\langle\alpha|\,\frac{1}{E-T+i\eta}\,|\beta\rangle &\Rightarrow \lim_{E\to\varepsilon_n}(E-\varepsilon_n)\frac{\delta(\boldsymbol{p}-\boldsymbol{p}')}{E-\frac{\boldsymbol{p}^2}{2m}+i\eta} \\ &= 0, \end{aligned} \tag{7.26}$$

whereas for the last term one obtains

$$\lim_{E\to\varepsilon_n}(E-\varepsilon_n)\times\sum_{\gamma\delta}\langle\alpha|\,\frac{1}{E-T+i\eta}\,|\gamma\rangle\,\langle\gamma|\,V\,|\delta\rangle\left\{\sum_m\frac{\langle\delta|m\rangle\langle m|\beta\rangle}{E-\varepsilon_m+i\eta}+...\right\}$$
$$=\sum_{\gamma\delta}\langle\alpha|\,\frac{1}{\varepsilon_n-T}\,|\gamma\rangle\,\langle\gamma|\,V\,|\delta\rangle\,\langle\delta|n\rangle\langle n|\beta\rangle$$
$$\Rightarrow\int d\boldsymbol{p}''\frac{1}{\varepsilon_n-\frac{\boldsymbol{p}^2}{2m}}\,\langle\boldsymbol{p}|\,V\,|\boldsymbol{p}''\rangle\,\langle\boldsymbol{p}''|n\rangle\langle n|\boldsymbol{p}'\rangle, \tag{7.27}$$

respectively. Collecting the two remaining terms, one has

$$\langle\boldsymbol{p}|n\rangle=\frac{1}{\varepsilon_n-\frac{\boldsymbol{p}^2}{2m}}\int d\boldsymbol{p}''\,\langle\boldsymbol{p}|\,V\,|\boldsymbol{p}''\rangle\,\langle\boldsymbol{p}''|n\rangle, \tag{7.28}$$

or, rearranging slightly and noting that $\langle\boldsymbol{p}|n\rangle=\phi_n(\boldsymbol{p})$, the momentum space wave function, one obtains

$$\frac{\boldsymbol{p}^2}{2m}\phi_n(\boldsymbol{p})+\int d\boldsymbol{p}''\,\langle\boldsymbol{p}|\,V\,|\boldsymbol{p}''\rangle\,\phi_n(\boldsymbol{p}'')=\varepsilon_n\phi_n(\boldsymbol{p}), \tag{7.29}$$

which corresponds to the Schrödinger equation in momentum space yielding the bound-state energies and corresponding momentum space eigenfunctions.

Instead of making the choice of the momentum representation one can also keep things general and collect the corresponding results from Eqs. (7.25)-(7.27) to obtain

$$\langle\alpha|n\rangle=\sum_{\gamma\delta}\langle\alpha|\,\frac{1}{\varepsilon_n-H_0}\,|\gamma\rangle\,\langle\gamma|\,V\,|\delta\rangle\,\langle\delta|n\rangle. \tag{7.30}$$

By multiplying this equation with $\langle\beta|\,(\epsilon_n-H_0)\,|\alpha\rangle$ and summing over α, one can reduce this equation to

$$\sum_\alpha\langle\beta|\,(\varepsilon_n-H_0)\,|\alpha\rangle\,\langle\alpha|n\rangle=\sum_\delta\langle\beta|\,V\,|\delta\rangle\,\langle\delta|n\rangle, \tag{7.31}$$

which is of course equivalent to

$$\varepsilon_n\langle\beta|n\rangle=\sum_\alpha\{\langle\beta|\,H_0\,|\alpha\rangle+\langle\beta|\,V\,|\alpha\rangle\}\,\langle\alpha|n\rangle, \tag{7.32}$$

the matrix form of the Schrödinger eigenvalue equation in the basis $\{|\alpha\rangle\}$.

Another useful exercise in anticipation of later many-body applications is to consider the issue of normalization. This is not a particularly illuminating problem for the usual case when V does not depend on the energy.

In the many-body problem we will, however, encounter similar sp propagator equations in which V has become energy dependent. If the potential V is energy-dependent, it is still possible to obtain the appropriate eigenvalue equation provided one assumes that V is well-behaved near ε_n. In the resulting eigenvalue equation V then appears at the eigenvalue ε_n as follows

$$\langle\alpha|n\rangle = \sum_{\gamma\delta} \langle\alpha| \frac{1}{\varepsilon_n - H_0} |\gamma\rangle \langle\gamma| V(\varepsilon_n) |\delta\rangle \langle\delta|n\rangle. \tag{7.33}$$

Near the discrete eigenvalue ε_n one can write the propagator as

$$G(\alpha,\beta;E \to \varepsilon_n) \Rightarrow \frac{\langle\alpha|n\rangle\langle n|\beta\rangle}{E-\varepsilon_n} + f_{\alpha\beta}(E), \tag{7.34}$$

where f is well-behaved near ε_n. The smooth behavior of $G^{(0)}$ and V near ε_n implies

$$\frac{G^{(0)}(E)V(E)}{E-\varepsilon_n} = \frac{G^{(0)}(\varepsilon_n)V(\varepsilon_n)}{E-\varepsilon_n} + \left.\frac{\partial G^{(0)}V}{\partial E}\right|_{\varepsilon_n} . \tag{7.35}$$

Inserting Eq. (7.34) in the propagator equation (7.17) using (7.35) and the smoothness of f one obtains

$$\begin{aligned}
\frac{\langle\alpha|n\rangle\langle n|\beta\rangle}{E-\varepsilon_n} + f_{\alpha\beta}(\varepsilon_n) &= G^{(0)}(\alpha,\beta;\varepsilon_n) \\
&+ \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E) \langle\gamma| V(E) |\delta\rangle \left\{ \frac{\langle\delta|n\rangle\langle n|\beta\rangle}{E-\varepsilon_n} + f_{\delta\beta}(\varepsilon_n) \right\} \\
&= G^{(0)}(\alpha,\beta;\varepsilon_n) + \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;\varepsilon_n) \langle\gamma| V(\varepsilon_n) |\delta\rangle \frac{\langle\delta|n\rangle\langle n|\beta\rangle}{E-\varepsilon_n} \\
&+ \sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;\varepsilon_n) \langle\gamma| V(\varepsilon_n) |\delta\rangle f_{\delta\beta}(\varepsilon_n) \\
&+ \sum_{\gamma\delta} \left.\frac{\partial G^{(0)}(\alpha,\gamma;E) \langle\gamma| V(E) |\delta\rangle}{\partial E}\right|_{\varepsilon_n} \langle\delta|n\rangle\langle n|\beta\rangle.
\end{aligned} \tag{7.36}$$

The first term on the left and the second on the right just represent the original eigenvalue equation (together these terms represent the singular terms of the propagator equation) and therefore are equal to each other. It is useful to multiply the remaining terms by $\langle n| (\varepsilon_n - H_0) |\alpha\rangle$ while summing over α. One can convince oneself that the terms containing f are then equal provided one also uses the alternative form of the eigenvalue equation that is obtained by considering the propagator equation in the form $G = G^{(0)} + G\ V\ G^{(0)}$ (see Eq. (7.19)). Eliminating these contributions, the rest of the terms can be further manipulated to obtain the normalization condition in the form

$$\sum_{\alpha} \langle n|\alpha\rangle\langle\alpha|n\rangle - \sum_{\alpha\beta} \langle n|\alpha\rangle\, \langle\alpha|\, \frac{\partial V(E)}{\partial E}\bigg|_{\varepsilon_n} |\beta\rangle\, \langle\beta|n\rangle = 1. \tag{7.37}$$

In the case of an energy-independent potential one naturally obtains the result

$$1 = \sum_{\alpha} |\langle\alpha|n\rangle|^2\,, \tag{7.38}$$

which can of course also be directly obtained by invoking the normalization of $|n\rangle$ and the completeness of the states $|\alpha\rangle$. In the exercises the steps outlined here for the more general energy-dependent case will be considered in more detail. It is useful to note that the normalization to 1 is related to the presence of $G^{(0)}$ in the propagator equation and the energy-independence of V. If V contains energy dependence one obtains additional terms contributing to the normalization as shown in Eq. (7.37).

7.4 Scattering theory using propagators

The elastic scattering process in free space is completely determined by one particular matrix element of the T-matrix. It is instructive to obtain this result explicitly using the propagator method. To this end one starts from Eq. (7.19) and uses its various incarnations to obtain the required analysis. Choosing a wave vector basis associated with the unperturbed Hamiltonian, $H_0 = T$, and assuming a spinless particle, the noninteracting propagator reads

$$G^{(0)}(\boldsymbol{k},\boldsymbol{k}';E) = \delta(\boldsymbol{k}-\boldsymbol{k}')\frac{1}{E - \hbar^2 k^2/2m + i\eta}. \tag{7.39}$$

Using this result in Eq. (7.19) one obtains

$$\begin{aligned} G(\boldsymbol{k},\boldsymbol{k}';E) &= G^{(0)}(\boldsymbol{k},\boldsymbol{k}';E) + G^{(0)}(\boldsymbol{k};E)\int d^3q \langle\boldsymbol{k}|V|\boldsymbol{q}\rangle G(\boldsymbol{q},\boldsymbol{k}';E) \\ &= G^{(0)}(\boldsymbol{k},\boldsymbol{k}';E) + G^{(0)}(\boldsymbol{k};E)\langle\boldsymbol{k}|T(E)|\boldsymbol{k}'\rangle G^{(0)}(\boldsymbol{k}';E), \end{aligned} \tag{7.40}$$

where

$$G^{(0)}(\boldsymbol{k},\boldsymbol{k}';E) \;=\; \delta(\boldsymbol{k}-\boldsymbol{k}')G^{(0)}(\boldsymbol{k};E) \tag{7.41}$$

is the noninteracting propagator. This second equality in Eq. (7.40) is particularly useful for the asymptotic analysis to be explored below. It is important to realize that the usual results from scattering theory are obtained in the coordinate representation. The relevant double Fourier transform of the propagator is given by

$$G(\boldsymbol{r},\boldsymbol{r}';E) \;=\; \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} G(\boldsymbol{k},\boldsymbol{k}';E) e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}. \tag{7.42}$$

The transform of the noninteracting propagator only involves one integration due to the presence of the δ-function in Eq. (7.41)

$$\begin{aligned} G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) &= \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}}\; e^{i\boldsymbol{k}\cdot\boldsymbol{r}} G^{(0)}(\boldsymbol{k},\boldsymbol{k}';E) e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \\ &= \int \frac{d^3k}{(2\pi)^3}\; e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} G^{(0)}(\boldsymbol{k};E). \end{aligned} \tag{7.43}$$

The result for Eq. (7.40) can then now be transformed to yield

$$\begin{aligned} G(\boldsymbol{r},\boldsymbol{r}';E) &= G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) \\ &\quad + \int d^3r_1 \int d^3r_2\; G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;E)\langle \boldsymbol{r}_1|V|\boldsymbol{r}_2\rangle G(\boldsymbol{r}_2,\boldsymbol{r}';E) \\ &= G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) \\ &\quad + \int d^3r_1 \int d^3r_2\; G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;E)\langle \boldsymbol{r}_1|T(E)|\boldsymbol{r}_2\rangle G^{(0)}(\boldsymbol{r}_2,\boldsymbol{r}';E). \end{aligned} \tag{7.44}$$

With this equation one can arrive at an asymptotic analysis and resulting definition of the cross section which is equivalent to a standard analysis involving the equation for the wave function.

To obtain the relation between the cross section and the propagator it is necessary to start with Eq. (7.45) and perform the Fourier transform of the noninteracting propagator (Eq. (7.39)) in Eq. (7.43). The on-shell wave vector k_0 is defined by

$$E \equiv \frac{\hbar^2 k_0^2}{2m}. \tag{7.45}$$

After performing the angular integrals and extending the integration limit in k to $-\infty$ one obtains (replacing E by k_0)

$$G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) = \frac{2m}{\hbar}\frac{1}{i|\boldsymbol{r}-\boldsymbol{r}'|}\frac{1}{8\pi^2}\int_{-\infty}^{\infty} dk\ k\frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}-e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}}{(k_0-k+i\eta)(k_0+k+i\eta)}$$
$$= \frac{2m}{\hbar}\frac{-1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}e^{ik_0|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{7.46}$$

where contour integration in the complex momentum plane has been used to obtain the last equality. When $r' \gg r$ one has the following result

$$k_0|\boldsymbol{r}-\boldsymbol{r}'| = k_0 r'\sqrt{1+\left(\frac{r}{r'}\right)^2-\frac{2\boldsymbol{r}\cdot\boldsymbol{r}'}{r'^2}} \approx k_0 r' - k_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}. \tag{7.47}$$

Using this result one can write Eq. (7.46) as

$$G^{(0)}(\boldsymbol{r},\boldsymbol{r}';k_0) \to -\frac{m}{2\pi\hbar}\frac{e^{ik_0 r'}}{r'}e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}}. \tag{7.48}$$

Substituting this result in the second part of Eq. (7.45) for both $r' \gg r$ and $r' \gg r_2$ demonstrates that G is separable and can be written as

$$G(\boldsymbol{r},\boldsymbol{r}';k_0) = -\frac{m}{2\pi\hbar}\frac{e^{ik_0 r'}}{r'}\psi(\boldsymbol{r};k_0) \tag{7.49}$$

in the asymptotic domain. By substituting this result in turn in Eq. (7.45) one obtains the standard integral equation for the wave function and the appropriate formulation for the asymptotic wave function to obtain the scattering amplitude

$$\psi(\boldsymbol{r};k_0) = e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}} + \int d^3r_1\int d^3r_2\ G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;k_0)\langle\boldsymbol{r}_1|V|\boldsymbol{r}_2\rangle\psi(\boldsymbol{r}_2;k_0)$$
$$= e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}}$$
$$+\int d^3r_1\int d^3r_2\ G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;k_0)\langle\boldsymbol{r}_1|T(k_0)|\boldsymbol{r}_2\rangle e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}_2}. \tag{7.50}$$

One may identify the origin of the motion in the direction of the negative z-axis, meaning that $\hat{\boldsymbol{r}}'$ points in that direction, so that $\boldsymbol{k} \equiv -k_0\hat{\boldsymbol{r}}'$ points into the positive z-direction. If one assumes that r is also much larger than the range of the potential, and, therefore much larger than any contributing value of r_1, one can use Eq. (7.48) again in the second part of Eq. (7.50) to identify the coefficient multiplying the outgoing spherical wave $e^{ik_0 r}/r$ as the scattering amplitude (while double Fourier transforming the T-matrix element back to momentum space)

$$f_{k_0}(\theta,\phi) = -\frac{4m\pi^2}{\hbar^2}\langle \boldsymbol{k}'|T(k_0)|\boldsymbol{k}\rangle, \tag{7.51}$$

where θ, ϕ denote the angles associated with the direction of $\hat{\boldsymbol{r}}$ and $\boldsymbol{k}' \equiv k_0\hat{\boldsymbol{r}}$ corresponds to the momentum of the detected motion in the direction $\hat{\boldsymbol{r}}$ with the same absolute value k_0 as the initial state. The differential cross section for the direction (θ, ϕ) is then simply the square of the scattering amplitude as given by Eq. (7.51)

$$\frac{d\sigma}{d\Omega} = |f_{k_0}(\theta,\phi)|^2 . \tag{7.52}$$

The present formulation is closely tailored to the conventional experimental situation where a collimated beam propagates along the z-axis characterized by a given energy or momentum toward a target situated at the origin. Detection then takes place in a particular direction away from the origin characterized by angles θ and ϕ. One can follow a similar derivation for a particle with spin to obtain the elastic scattering amplitude ($|\boldsymbol{p}_f| = |\boldsymbol{p}_i|$)

$$f_{m_f,m_i}(\theta,\phi) = -\frac{m\hbar}{2\pi}(2\pi)^3 \langle \boldsymbol{p}_f m_f|\, T(E = \frac{\boldsymbol{p}_i^2}{2m})\, |\boldsymbol{p}_i m_i\rangle \tag{7.53}$$

with θ and ϕ giving the direction of $\boldsymbol{p}_f$ with respect to the z-axis which is defined by $\boldsymbol{p}_i$. The cross section is obtained from the usual relation

$$\frac{d\sigma^{m_f,m_i}}{d\Omega} = |f_{m_f,m_i}(\theta,\phi)|^2. \tag{7.54}$$

7.4.1 *Partial Waves and Phase Shifts*

Often the interaction is of short range. When this is the case, it is invariably useful to analyze the scattering process in an angular momentum basis since only a limited set of ℓ-values will contribute. The appropriate basis tranformation from momentum space to an angular momentum basis is given by

$$|\boldsymbol{k}\rangle = \sum_{\ell m_\ell} |k\ell m_\ell\rangle\, \langle \ell m_\ell|\hat{\boldsymbol{k}}\rangle = \sum_{\ell m_\ell} |k\ell m_\ell\rangle\, Y^*_{\ell m_\ell}(\hat{\boldsymbol{k}}). \tag{7.55}$$

In this basis the noninteracting propagator is given by

$$G^{(0)}(k\ell m_\ell, k'\ell' m_{\ell'}; E) = \frac{\delta(k-k')}{k^2}\delta_{\ell\ell'}\delta_{m_\ell m_{\ell'}}\frac{1}{E - \hbar^2k^2/2m + i\eta}$$

$$= \frac{\delta(k-k')}{k^2}\delta_{\ell\ell'}\delta_{m_\ell m_{\ell'}}G^{(0)}(k;E). \qquad (7.56)$$

Since the energy has no angular dependence, the energy denominator is the same as in the wave vector basis (7.39) Expressing Eq. (7.19) in this angular momentum basis and assuming that the interaction is rotationally invariant (and therefore does not couple different ℓ-values) one has

$$\begin{aligned} G_\ell(k,k';E) &= \frac{\delta(k-k')}{k^2}G^{(0)}(k;E) \qquad (7.57)\\ &+ G_\ell(k;E)\int_0^\infty dq q^2\langle k|V^\ell|q\rangle G_\ell(q,k';E)\\ &= \frac{\delta(k-k')}{k^2}G^{(0)}(k;E) + G^{(0)}(k;E)\langle k|T^\ell(E)|k'\rangle G^{(0)}(k';E). \end{aligned}$$

The equation for the effective interaction or T-matrix can be written in this basis as

$$\langle k|T^\ell(E)|k'\rangle = \langle k|V^\ell|k'\rangle + \int_0^\infty dq\ q^2\langle k|V^\ell|q\rangle G^{(0)}(q;E)\langle q|T^\ell(E)|k'\rangle. \qquad (7.58)$$

The coordinate space version of Eq. (7.58) is obtained by a double Fourier-Bessel transform

$$G_\ell(r,r';E) = \frac{2}{\pi}\int_0^\infty dk\ k^2\int_0^\infty dk'\ k'^2\ j_\ell(kr)j_{\ell'}(k'r')G_\ell(k,k';E), \quad (7.59)$$

which involves the transformation from angular momentum states with momentum to angular momentum states with position involving the spherical Bessel function

$$\langle k\ell m_\ell|r\ell' m_{\ell'}\rangle = \delta_{\ell\ell'}\delta_{m_\ell m_{\ell'}}\sqrt{\frac{2}{\pi}}j_\ell(kr). \qquad (7.60)$$

The corresponding result for the noninteracting part of the propagator, represented by the first term in Eq. (7.58), reduces to one integral on account of the delta-function which conserves relative momentum

$$G_\ell^{(0)}(r,r';E) = \frac{2}{\pi}\int_0^\infty dk\ k^2\ j_\ell(kr)j_\ell(kr')G^{(0)}(k;E). \qquad (7.61)$$

The Fourier-Bessel transform of Eq. (7.58) has the following form

$$\begin{aligned} G_\ell(r,r';E) &= G_\ell^{(0)}(r,r';E) + \int_0^\infty dr_1 r_1^2\int_0^\infty dr_2 r_2^2\\ &\times G_\ell(r,r_1;E)\langle r_1|V^\ell|r_2\rangle G_\ell(r_2,r';E) \end{aligned}$$

$$= G_\ell^{(0)}(r, r'; E) + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2$$
$$\times G_\ell^{(0)}(r, r_1; E) \langle r_1 | T^\ell(E) | r_2 \rangle G_\ell^{(0)}(r_2, r'; E). \qquad (7.62)$$

When the interaction V is local in coordinate space, only one integral in the first equality remains. The second equality can be used to study the asymptotic behavior of the propagator outside the range of the interaction. The integral in Eq. (7.61) can be performed analytically by employing contour integration in the complex momentum plane as discussed in the book by Gottfried. The spherical Bessel function are well-behaved so all the singularities are contained in the denominator. Consider $r' > r$, then one may replace

$$j_\ell(kr') = \frac{1}{2}\left[h_\ell(kr') + h_\ell^*(kr')\right], \qquad (7.63)$$

involving the spherical Hankel functions. One can convince oneself that the term involving $j_\ell h_\ell$ decreases exponentially in the upper half k-plane, allowing the contour to be closed in the upper half-plane. The term involving $j_\ell h_\ell^*$, similarly, requires a contour in the lower half-plane. One then obtains

$$G_\ell^{(0)}(r, r'; k_0) = -ik_0 \frac{2m}{\hbar} j_\ell(k_0 r_<) h_\ell(k_0 r_>). \qquad (7.64)$$

The coordinate argument in the spherical Hankel function must be the larger of r and r' and is denoted by $r_>$ while the argument of the spherical Bessel function is the smaller and denoted by $r_<$. For the current analysis it will be assumed that the interaction has a finite range, $\langle r | V^\ell | r' \rangle = 0$ for r, r' larger than some r_0. Substituting Eq. (7.64) in the second part of Eq. (7.62) for $r' > r$ and $r' > r_0$ yields

$$\begin{aligned} G_\ell(r, r'; k_0) &= -ik_0 \frac{2m}{\hbar} j_\ell(k_0 r) h_\ell(k_0 r') \\ &+ \frac{1}{\hbar}\int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2 \; G_\ell^{(0)}(r, r_1; k_0) \langle r_1 | T^\ell(k_0) | r_2 \rangle \\ &\times \left(-ik_0 \frac{2m}{\hbar}\right) j_\ell(k_0 r_2) h_\ell(k_0 r') \\ &= -ik_0 \frac{2m}{\hbar} \psi_\ell(r; k_0) h_\ell(k_0 r'), \end{aligned} \qquad (7.65)$$

where

$$\psi_\ell(r; k_0) = j_\ell(k_0 r) \qquad (7.66)$$

$$+ \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2 \; G_\ell^{(0)}(r, r_1; k_0) \langle r_1 | T^\ell(k_0) | r_2 \rangle j_\ell(k_0 r_2),$$

including the replacement of E by k_0. This result demonstrates that under the given conditions the propagator separates as a product of a function r and a function of r'. This result can be substituted into the first part of Eq. (7.62) to obtain the relevant integral equation for the wave function ψ (under the condition that $r' > r_0$)

$$\psi_\ell(r; k_0) = j_\ell(k_0 r) + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2 \; G_\ell^{(0)}(r, r_1; k_0) \langle r_1 | V^\ell | r_2 \rangle \psi_\ell(r_2; k_0), \tag{7.67}$$

which can be found in standard textbooks (see *e.g.* Gottfried for the case of a local potential). It is derived here to demonstrate the relation between the propagator and the wave function.

The asymptotic analysis of the propagator can be performed by using Eq. (7.64) in Eq. (7.62) under the assumption that the propagator will be considered for $r < r'$ while both these coordinates are larger than r_0, the range of the interaction. Values of r_1 and r_2 in Eq. (7.62) larger than r_0 yield no contributions to the integral. As a result, the effective interaction, T, has a range similar to the one of the bare interaction V. Using the relation between spherical Bessel and Hankel functions (7.63), one obtains the asymptotic behavior of the propagator from the second part of Eq. (7.62) in the following form

$$\begin{aligned} G_\ell(r, r'; k_0) &\to -i \left(\frac{m}{\hbar}\right) k_0 h_\ell(k_0 r') \Big\{ h_\ell^*(k_0 r) + h_\ell(k_0 r) \big[1 - 4i \frac{m}{\hbar^2} k_0 \\ &\quad \times \int_0^\infty dr_1 \; r_1^2 \; \int_0^\infty dr_2 \; r_2^2 \; \langle r_1 | T^\ell(k_0) | r_2 \rangle j_\ell(k_0 r_1) j_\ell(k_0 r_2) \big] \Big\} \\ &= -i \frac{m}{\hbar} k_0 h_\ell(k_0 r') \\ &\quad \times \left\{ h_\ell^*(k_0 r) + h_\ell(k_0 r) \left[1 - 2\pi i \left(\frac{m k_0}{\hbar^2} \right) \langle k_0 | T^\ell(k_0) | k_0 \rangle \right] \right\}. \end{aligned} \tag{7.68}$$

In the last step of Eq. (7.69) one can return to the on-shell matrix element of the T-matrix in momentum space which completely determines the outcome of the scattering process. The term in square brackets corresponds to the S-matrix element in terms of which one can define the phase shift

$$\langle k_0 | S^\ell(k_0) | k_0 \rangle = \left[1 - 2\pi i \left(\frac{m k_0}{\hbar^2} \right) \langle k_0 | T^\ell(k_0) | k_0 \rangle \right] \equiv e^{2i\delta_\ell}. \tag{7.69}$$

This result can be represented by

$$\tan\delta_\ell = \frac{\mathrm{I}m\langle k_0|T^\ell(k_0)|k_0\rangle}{\mathrm{R}e\langle k_0|T^\ell(k_0)|k_0\rangle}, \tag{7.70}$$

which explicitly shows that a nonzero imaginary part of the effective interaction is required to obtain a nonvanishing phase shift. In turn, this imaginary part of the interaction only appears for energies where the noninteracting propagator has a nonvanishing imaginary part. For the scattering this corresponds to all positive energies. By substituting the explicit form of the spherical Hankel functions for $\ell = 0$ in Eq. (7.69) one can construct the asymptotic propagator for the s-wave channel explicitly

$$G_s(r,r';k_0) \to -\frac{2m}{k_0\hbar}\frac{1}{rr'}e^{i(k_0r'+\delta_s)}\sin(k_0r+\delta_s). \tag{7.71}$$

The standard result for the asymptotic wave function is contained in this equation and the imaginary part of Eq. (7.71) is simply the product of these wave functions as a function of r and r', respectively. It is useful to write the scattering amplitude in terms of the on-shell T-matrix elements or phase shift

$$\begin{aligned} f(\theta,\phi) &= \sum_l \frac{2l+1}{k_0}\left\{\frac{-mk_0\pi}{\hbar^2}\right\}\langle k_0|T^\ell(k_0)|k_0\rangle P_\ell(\cos\theta) \\ &= \sum_\ell \frac{2\ell+1}{k_0}e^{i\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta). \end{aligned} \tag{7.72}$$

With this result one can construct the differential cross section. For the total cross section one has

$$\sigma_{tot} = \frac{4\pi}{k_0^2}\sum_\ell(2\ell+1)\sin^2\delta_\ell. \tag{7.73}$$

7.5 Exercises

(1) Consider the second-order diagram contributing to G. Perform the inverse Fourier transform to obtain this contribution as a function of the time difference $t - t'$.
(2) Construct all diagrammatic representations of Eqs. (7.19) and (7.20).
(3) Work out the details of the normalization of the state $|n\rangle$ in the case of an energy-dependent potential $V(E)$ following the outline given below Eq. (7.36) and obtain Eq. (7.37).

(4) Perform all the operations that lead to Eq. (7.64).

(5) Extend the formalism discussed in Sec. 7.4.1 to the case of a spin 1/2 fermion which also experiences a spin-orbit potential as discussed in Sec. 3.3.