Comments on section 6.1 of [SN]

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1 The physical system and how we model it

In a scattering experiment, one shoots a beam of particles onto a target, and detectors positioned far from the target and at definite angles compared to the input beam measure the rate at which the incoming particles are scattered into that direction. The target is modeled by a potential V, which goes to zero as the distance to the target is increased. Ideally, one should describe the incoming particles as wave packets, but this is difficult to do. We hence consider a simpler description, in which the incoming particles are described by a plane wave that fills all of space. This is a reasonable description if the wave packets of the particles are broad compared to the target. Most of the time, we consider space to be a cube with side length L for convenience, where L should be taken to infinity at the end of the computations. We do this to describe Hilbert space in terms of a discrete set of states rather than a continuum of states. The incoming plane wave has been there for all times, and hence the problem is time independent, if the potential is time independent. We can therefore solve it by solving the time independent Schrödinger equation. We discuss this further below. The book chooses instead to solve the problem with the machinery of time dependent perturbation theory, because this approach can also be applied when the potential is time dependent.

2 The Lippmann-Schwinger equation

When the scattering potential V is independent of time, we are actually solving a time independent problem, and we can do this by solving the time independent Schrödinger equation

$$H_0|\psi\rangle + V|\psi\rangle = E|\psi\rangle, \qquad H_0 = \frac{\mathbf{p}^2}{2m}, \tag{1}$$

where H_0 is the Hamiltonian of a free particle, i.e. $\mathbf{p}$ is the momentum operator, and m is the mass of the incoming particle. We rearrange this equation into

$$V|\psi\rangle = (E - H_0)|\psi\rangle. \tag{2}$$

The time independent Schrödinger equation has as many solutions as the dimension of the Hilbert space. Here, we are, however, only interested in one solution $|\psi^{(+)}\rangle$, namely the solution that reduces to the incoming plane wave $|\mathbf{k}\rangle$ when $V \to 0$. Since the target in the scattering process is here assumed to be a potential and not by itself a quantum system or drive, the target cannot change its energy. We are hence describing an elastic scattering process, in which the scattered particle has the same energy as the incoming particle to fulfil energy conservation, so the energy of the sought solution must be $E = \hbar^2 k^2/(2m) \equiv E_i$.

In a moment, we will divide by $(E_i - H_0)$, so to avoid singularities, we regularize the Schrödinger equation by modifying the energy E_i of the state $|\psi^{(+)}\rangle$ into $E_i + i\hbar\varepsilon$, i.e.

$$V|\psi^{(+)}\rangle = (E_i - H_0 + i\hbar\varepsilon)|\psi^{(+)}\rangle, \tag{3}$$

where $\varepsilon \to 0$. This allows us to write the sought solution as

$$|\psi^{(+)}\rangle = |\mathbf{k}\rangle + \frac{1}{E_i - H_0 + i\hbar\varepsilon} V|\psi^{(+)}\rangle, \tag{4}$$

eqn. 6.29 (Lippmann-Schwinger eqn.)

where

$$\frac{1}{E_i - H_0 + i\hbar\varepsilon} \equiv (E_i - H_0 + i\hbar\varepsilon)^{-1}. \tag{5}$$

That (4) is indeed a solution to (2) can be seen by applying $(E_i - H_0 + i\hbar\varepsilon)$ to (4) from the left, taking $\varepsilon \to 0$, and noting that $(E_i - H_0)|\mathbf{k}\rangle = 0$. Note that equation (4) is the same equation as (6.29) in [SN], and this equation is called the Lippmann-Schwinger equation. Note also that we can replace every $|\psi^{(+)}\rangle$ appearing on the right hand side of (4) by the right hand side of (4) to get an infinite series expansion for $|\psi^{(+)}\rangle$. The nth term in that expansion contains V a total of $n-1$ times, so if V is small, the expansion can be truncated to a reasonable accuracy. Once we have found $|\psi^{(+)}\rangle$, we can compute, for instance, the particle density in space the usual way, namely as $|\langle\mathbf{x}|\psi^{(+)}\rangle|^2$. We can also consider other bases, such as the occupation of different momentum eigenstates or spherical waves.

Finally, we note that we could alternatively have regularized by taking $E_i \to E_i - i\hbar\varepsilon$ rather than $E_i \to E_i + i\hbar\varepsilon$. We denote the corresponding state by $|\psi^{(-)}\rangle$. We hence write

$$|\psi^{(\pm)}\rangle = |\mathbf{k}\rangle + \frac{1}{E_i - H_0 \pm i\hbar\varepsilon} V|\psi^{(\pm)}\rangle. \tag{6}$$

At this moment, the physical significance of taking $E_i \to E_i \pm i\hbar\varepsilon$ is not clear. The meaning will become clear later in the course.

3 Time dependent perturbation theory

We now investigate the same problem from the point of view of time dependent perturbation theory. There is still no time dependence in the problem. The potential has been there forever, so we should take $t_0 \to -\infty$.

From our discussions of chapter 5 of [SN], the probability amplitude for transfer from the initial momentum eigenstate $|i\rangle = |\mathbf{k}\rangle$ to some final momentum eigenstate $|n\rangle$ is given by

$$\langle n|U_I(t,-\infty)|i\rangle = \delta_{ni} - \frac{i}{\hbar}\sum_m V_{nm}\int_{-\infty}^{t} e^{i\omega_{nm}t'}\langle m|U_I(t',-\infty)|i\rangle dt', \tag{7}$$

where we have taken V_{nm} outside the integral as V_{nm} is time independent. We will solve (7) by guessing the solution. Our guess is

$$\langle m|U_I(t,-\infty)|i\rangle = \delta_{mi} - \frac{i}{\hbar}T_{mi}\int_{-\infty}^{t} e^{i\omega_{mi}t'}dt', \tag{8}$$

where we do not yet know what T_{ni} is, but we will take T_{ni} to be time independent. [SN] states that (8) is a definition of T_{ni} with T_{ni} time independent. If T_{ni} is time independent, however, (8) already fixes the time dependence of $\langle n|U_I(t,-\infty)|i\rangle$. (8) is hence more appropriately seen as a guess for a solution of (7). Inserting (8) into (7), we obtain

$$\begin{aligned}\delta_{ni} - \frac{i}{\hbar}T_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'}dt' &= \delta_{ni} - \frac{i}{\hbar}V_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'}dt' \\ &\quad - \frac{1}{\hbar^2}\sum_m V_{nm}T_{mi}\int_{-\infty}^{t} e^{i\omega_{nm}t'}\int_{-\infty}^{t'} e^{i\omega_{mi}t''}dt''dt'. \end{aligned}\tag{9}$$

We are running into trouble here, because ω_{ni} is zero, and $\int_{-\infty}^{t} dt'$ is infinite. We solve this problem through the same regularization procedure as above, namely by taking $E_i \to E_i + i\hbar\varepsilon$ and hence $\omega_{mi} \to \omega_{mi} - i\varepsilon$. This modifies (9) to

$$\begin{aligned}\delta_{ni} - \frac{i}{\hbar}T_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' &= \delta_{ni} - \frac{i}{\hbar}V_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' \\ &\quad - \frac{1}{\hbar^2}\sum_m V_{nm}T_{mi}\int_{-\infty}^{t} e^{i\omega_{nm}t'}\int_{-\infty}^{t'} e^{i\omega_{mi}t''+\varepsilon t''}dt''dt'. \end{aligned}\tag{10}$$

Canceling out δ_{ni} and doing one of the integrals, we get

$$\begin{aligned}-\frac{i}{\hbar}T_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' &= -\frac{i}{\hbar}V_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' \\ &\quad - \frac{1}{\hbar^2}\sum_m V_{nm}T_{mi}\int_{-\infty}^{t} e^{i\omega_{nm}t'}\frac{e^{i\omega_{mi}t'+\varepsilon t'}}{i\omega_{mi}+\varepsilon}dt'. \end{aligned}\tag{11}$$

Noting that $\omega_{nm} + \omega_{mi} = \omega_{ni}$, this simplifies to

$$\begin{aligned}-\frac{i}{\hbar}T_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' &= -\frac{i}{\hbar}V_{ni}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' \\ &\quad - \frac{1}{\hbar^2}\sum_m V_{nm}T_{mi}\frac{1}{i\omega_{mi}+\varepsilon}\int_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt'. \end{aligned}\tag{12}$$

and hence

$$T_{ni} = V_{ni} + \sum_m V_{nm} T_{mi} \frac{1}{-\hbar\omega_{mi} + i\hbar\varepsilon}. \tag{13}$$

Since $H_0|m\rangle = E_m|m\rangle$, this can also be written as

$$\langle n|T|i\rangle = \langle n|V|i\rangle + \sum_m \langle n|V \frac{1}{E_i - H_0 + i\hbar\varepsilon}|m\rangle\langle m|T|i\rangle, \tag{14}$$

which is the matrix elements of the operator

$$T = V + V\frac{1}{E_i - H_0 + i\hbar\varepsilon}T. \tag{15}$$

In conclusion, (8) is indeed a solution to (7), provided we choose T as in (15).

4 $T|\mathbf{k}\rangle = V|\psi^{(+)}\rangle$

Let us apply T to the incoming plane wave $|i\rangle = |\mathbf{k}\rangle$, which gives

$$T|\mathbf{k}\rangle = V|\mathbf{k}\rangle + V\frac{1}{E_i - H_0 + i\hbar\varepsilon}T|\mathbf{k}\rangle. \tag{16}$$

If we apply V to the Lippmann-Schwinger equation, we get

$$V|\psi^{(+)}\rangle = V|\mathbf{k}\rangle + V\frac{1}{E_i - H_0 + i\hbar\varepsilon}V|\psi^{(+)}\rangle. \tag{17}$$

If we do the usual trick of inserting the right hand side on the right hand side again and again, we see that $T|\mathbf{k}\rangle$ and $V|\psi^{(+)}\rangle$ are given by the same infinite series. Therefore

$$T|\mathbf{k}\rangle = V|\psi^{(+)}\rangle. \tag{18}$$

References

[SN] J. J. Sakurai and J. Napolitano, Modern Quantum Mechanics, third edition, Cambridge University Press (2021).