4

Green's Functions and Perturbation Theory

Summary. The problem of finding the eigenvalues and eigenfunctions of a Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ can be solved in three steps: 1) Calculate the Green's function $G_0(z)$ corresponding to $\mathcal{H}_0$. 2) Express $G(z)$ as a perturbation series in terms of $G_0(z)$ and $\mathcal{H}_1$, where $G(z)$ is the Green's function associated with $\mathcal{H}$. 3) Extract from $G(z)$ information about the eigenvalues and eigenfunctions of $\mathcal{H}$.

4.1 Formalism

4.1.1 Time-Independent Case

In this chapter we consider the very important and common case where the one-particle Hamiltonian $\mathcal{H}$ can be separated into an unperturbed part $\mathcal{H}_0$ and a perturbation $\mathcal{H}_1$

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \ . \tag{4.1}$$

It is implicitly assumed that $\mathcal{H}_0$ is such that its eigenvalues and eigenfunctions can be easily obtained. The question is to determine the eigenvalues and eigenfunctions of $\mathcal{H}$. Very often this goal is achieved by taking the following indirect path:

1. Determine first the Green's function G_0 associated with the unperturbed part $\mathcal{H}_0$.
2. Express the Green's function G associated with the total Hamiltonian $\mathcal{H}$ in terms of G_0 and $\mathcal{H}_1$.
3. Obtain information about the eigenvalues and eigenfunctions of $\mathcal{H}$ from G.

Step 3 above has been examined in detail in Chap. 1 and Sect. 3.1. The implementation of step 1 depends on $\mathcal{H}_0$. For the very common and important case where $\mathcal{H}_0 = p^2/2m$, G_0 has been obtained in Sect. 3.2. In the next chapter a whole class of $\mathcal{H}_0$s will be introduced, and the corresponding G_0s will be calculated. In the present section we examine in some detail step 2, i.e., how G can be expressed in terms of G_0 and $\mathcal{H}_1$.

The Green's functions $G_0(z)$ and $G(z)$ corresponding to $\mathcal{H}_0$ and $\mathcal{H}$, respectively, are

$$G_0(z) = (z - \mathcal{H}_0)^{-1} \qquad \text{and} \tag{4.2}$$
$$G(z) = (z - \mathcal{H})^{-1} \ . \tag{4.3}$$

Using (4.1) and (4.2) we can rewrite (4.3) as follows:

$$\begin{aligned} G(z) &= (z - \mathcal{H}_0 - \mathcal{H}_1)^{-1} = \left\{(z - \mathcal{H}_0)\left[1 - (z - \mathcal{H}_0)^{-1}\mathcal{H}_1\right]\right\}^{-1} \\ &= \left[1 - (z - \mathcal{H}_0)^{-1}\mathcal{H}_1\right]^{-1}(z - \mathcal{H}_0)^{-1} \\ &= [1 - G_0(z)\mathcal{H}_1]^{-1} G_0(z) \ . \end{aligned} \tag{4.4}$$

Expanding the operator $(1 - G_0\mathcal{H}_1)^{-1}$ in power series we obtain

$$G = G_0 + G_0\mathcal{H}_1 G_0 + G_0\mathcal{H}_1 G_0 \mathcal{H}_1 G_0 + \cdots \ . \tag{4.5}$$

Equation (4.5) can be written in a compact form

$$G = G_0 + G_0\mathcal{H}_1\left(G_0 + G_0\mathcal{H}_1 G_0 + \cdots\right) = G_0 + G_0\mathcal{H}_1 G \tag{4.6}$$

or

$$G = G_0 + \left(G_0 + G_0\mathcal{H}_1 G_0 + \cdots\right)\mathcal{H}_1 G_0 = G_0 + G\mathcal{H}_1 G_0 \ . \tag{4.7}$$

In the $\boldsymbol{r}$-representation, (4.6) becomes

$$\begin{aligned} G(\boldsymbol{r}, \boldsymbol{r}'; z) &= G_0(\boldsymbol{r}, \boldsymbol{r}'; z) \\ &\quad + \int \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 G_0(\boldsymbol{r}, \boldsymbol{r}_1; z)\mathcal{H}_1(\boldsymbol{r}_1, \boldsymbol{r}_2) G(\boldsymbol{r}_2, \boldsymbol{r}'; z) \ . \end{aligned} \tag{4.6$'$}$$

Usually $\mathcal{H}_1(\boldsymbol{r}_1, \boldsymbol{r}_2)$ has the form $\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) V(\boldsymbol{r}_1)$; then (4.6$'$) becomes

$$\begin{aligned} G(\boldsymbol{r}, \boldsymbol{r}'; z) &= G_0(\boldsymbol{r}, \boldsymbol{r}'; z) \\ &\quad + \int \mathrm{d}\boldsymbol{r}_1 G_0(\boldsymbol{r}, \boldsymbol{r}_1; z) V(\boldsymbol{r}_1) G(\boldsymbol{r}_1, \boldsymbol{r}'; z) \ , \end{aligned} \tag{4.8}$$

i.e., $G(\boldsymbol{r}, \boldsymbol{r}'; z)$ satisfies a linear inhomogeneous integral equation with a kernel $G_0(\boldsymbol{r}, \boldsymbol{r}_1; z) V(\boldsymbol{r}_1)$. Equation (4.7) can be written also in a similar form. If we use the $\boldsymbol{k}$-representation, we can rewrite (4.6) as follows:

$$G(\boldsymbol{k}, \boldsymbol{k}'; z) = G_0(\boldsymbol{k}, \boldsymbol{k}'; z) + \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2} G_0(\boldsymbol{k}, \boldsymbol{k}_1; z)\mathcal{H}_1(\boldsymbol{k}_1, \boldsymbol{k}_2) G(\boldsymbol{k}_2, \boldsymbol{k}'; z) \ . \tag{4.9}$$

Taking into account that $\langle \boldsymbol{r} \,|\, \boldsymbol{k} \rangle = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}/\sqrt{\Omega}$ and that

$$\sum_{\boldsymbol{k}} = \Omega \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d} \ , \tag{4.10}$$