3.2 Introduction to Green's functions

Green's functions appear naturally in many perturbative calculations. We have seen an example in Sections 3.1.6 and 3.1.7, where $\langle a^+(x)a(y)\rangle$ may be interpreted as *equal-time* Green's functions. However, if we choose to extend the calculations of Section 3.1.7 to higher orders in interaction, we would need to introduce time-dependent (or frequency-dependent) Green's functions. Indeed, at higher orders, we cannot neglect noncommutativity between H and V in Eq. (3.1.41). The expansion of the operator exponent, to any order, is given by:

$$e^{-\beta(H_0+V)} = e^{-\beta H_0} + \int_0^\beta d\tau_1\, e^{-(\beta-\tau_1)H_0}(-V)e^{-\tau_1 H_0} + \iint_{0<\tau_1<\tau_2<\beta} d\tau_1\, d\tau_2\, e^{-(\beta-\tau_2)H_0}(-V)e^{-(\tau_2-\tau_1)H_0}(-V)e^{-\tau_1 H_0} + \dots \qquad (3.2.1)$$

The same type of formula is also valid for time evolution in quantum mechanics (by replacing imaginary time τ by real time t):

$$e^{-it(H_0+V)} = e^{-itH_0} + \int_0^t dt_1\, e^{-i(t-t_1)H_0}(-iV)e^{-it_1 H_0} + \iint_{0<t_1<t_2<t} dt_1\, dt_2\, e^{-i(t-t_2)H_0}(-iV)e^{-i(t_2-t_1)H_0}(-iV)e^{-it_1 H_0} + \dots \qquad (3.2.2)$$

This series can be conveniently represented graphically (Fig. 8). It has the meaning of the interaction intervening at the moments t_1, t_2, etc. during the evolution of the system.

3.2.1 Green's functions in quantum mechanics

Before introducing Green's functions in the second-quantized formalism, we discuss briefly their application in quantum mechanics. We define the Green's function as the propagator (evolution operator)

$$G(x',x,t) = -i\langle x'|e^{-itH}|x\rangle\, \theta(t)\,, \qquad (3.2.3)$$

where $\theta(t)=1$ for $t>0$ and $\theta(t)=0$ for $t<0$ (the factor $-i$ is introduced for convenience to simplify further formulas). Such a definition is usually called the *retarded* Green's function. The Green's function can be represented either in the coordinate or in the momentum space (related by a Fourier transformation) and either in the time or in the frequency space (again, related by a Fourier transformation). For example, passing to the frequency representation gives

$$G_\omega(x',x) = \int dt\, e^{i(\omega+i0)t} G(x',x,t) = \langle x'|\frac{1}{\omega - H + i0}|x\rangle\,. \qquad (3.2.4)$$

Figure 8: Perturbation series for the Green's function.

If H is a free-particle Hamiltonian ($H = \varepsilon_k$ in the momentum representation), then it is convenient to represent the Green's function also in the momentum representation, where it becomes diagonal:

$$G_\omega(k', k) = \iint d^3x'\, d^3x\, G_\omega(x', x) e^{-ik'x'+ikx} = (2\pi)^3 \delta(k-k')\, G_\omega(k)\,, \tag{3.2.5}$$

where

$$G_\omega(k) = \frac{1}{\omega - \varepsilon_k + i0}\,. \tag{3.2.6}$$

The appearance of such Green's functions can be understood already from the perturbation theory in quantum mechanics. If we consider a Schroedinger equation with a perturbation:

$$(H_0 + V)\Psi = E\Psi\,, \tag{3.2.7}$$

then we may formally solve it perturbatively by rewriting

$$\Psi = (E - H_0)^{-1} V\Psi\,. \tag{3.2.8}$$

The inverse $(E - H_0)^{-1}$ coincides with our above definition of the Green's function: we can also write it as an operator

$$G = \frac{1}{E - H_0 + i0} \tag{3.2.9}$$

The perturbative series for Ψ can be constructed iteratirvely

$$\Psi = \Psi_0 + \Psi_1 + \ldots \tag{3.2.10}$$

starting with Ψ_0 (an eigenstate of H_0 at energy E) and solving iteratively:

$$(E - H_0)\Psi_{n+1} = V\Psi_n \qquad \Rightarrow \qquad \Psi_{n+1} = (E - H_0)^{-1} V\Psi_n\,. \tag{3.2.11}$$

As a result, we get the perturbative series

$$\Psi = (1 + GV + GVGV + \ldots)\,\Psi_0\,, \tag{3.2.12}$$

where we again recognize the series of the type shown in Fig. 8.

Yet another way to obtain the same series is to expand the full Green's function:

$$\begin{aligned}\tilde{G} &= \frac{1}{E - (H_0 + V)} \\ &= \frac{1}{E - H_0} + \frac{1}{E - H_0} V \frac{1}{E - H_0} + \frac{1}{E - H_0} V \frac{1}{E - H_0} V \frac{1}{E - H_0} + \ldots\,,\end{aligned} \tag{3.2.13}$$

which is the operator counterpart of the usual power series:

$$\frac{1}{a - \epsilon} = \frac{1}{a} + \frac{1}{a^2}\epsilon + \frac{1}{a^3}\epsilon^2 + \ldots \tag{3.2.14}$$

(Note: the order of operators in the right-hand side of (3.2.13) is important!) We can see that it again reduces to the same series in Fig. 8.

Figure 9: Left: A sketch of the experimental observation in the paper of Kanisawa et al. Friedel oscillations of the local density of states are observed around impurities. x is the observation point, y is the position of the impurity. Right: the diagram representing the first-order correction to the density of states due to the impurity potential.

3.2.2 Application: Density-of-states oscillations around an impurity

Consider the experiment described in the paper K. Kanisawa et al, Phys. Rev. Lett. **86**, 3384 (2001): the local density of states at a given energy is measured around an impurity in a two-dimensional electron gas (Fig. 9). We can express this local density of states in terms of the retarded Green's function as

$$\rho_\omega(x) = -\frac{1}{\pi}\,\mathrm{Im}\,\tilde{G}_\omega(x,x)\,, \tag{3.2.15}$$

where $\tilde{G}$ is the full Green's function (3.2.13) To the first order in the impurity potential $V(x)$, the distortion of the local density of states is given by

$$\delta\rho_\omega(x) = -\frac{1}{\pi}\,\mathrm{Im}\int d^2y\,G_\omega(x,y)\,V(y)\,G_\omega(y,x)\,. \tag{3.2.16}$$

By approximating the potential to be a delta function $V(y) = V_0\,\delta(y)$, we find

$$\delta\rho_\omega(R) = -\frac{V_0}{\pi}\,\mathrm{Im}[G_\omega(R)]^2\,, \tag{3.2.17}$$

where $R = |x|$ is the distance from the impurity. The Green's function of a free particle, in turn, can be expressed as

$$G_\omega(x) = \int \frac{1}{\omega - (k^2/2m) + i0}\,e^{ikx}\,\frac{d^2k}{(2\pi)^2}\,. \tag{3.2.18}$$

The two last equations solve the problem in principle. The analytic treatment of integrals is complicated in 2D, but we can simplify it in the limit $k_\omega R \gg 1$, where $k_\omega = (2m\omega)^{1/2}$. Performing first the integrals over the angular degrees of freedom in (3.2.18), we find

$$G_\omega(R) = \int_0^\infty \frac{kJ_0(kR)}{\omega - (k^2/2m) + i0}\,\frac{dk}{2\pi}\,, \tag{3.2.19}$$

where J_0 is the Bessel function:

$$J_0(x) = \int_0^{2\pi} \frac{d\varphi}{2\pi}\,e^{ix\cos\varphi}\,. \tag{3.2.20}$$

At $kR \gg 1$, the asymptotic behavior of $J_0(kR)$ is

$$J_0(kR) \approx \sqrt{\frac{2}{\pi kR}} \cos\left(kR - \frac{\pi}{4}\right) \tag{3.2.21}$$

The main contribution to the integral (3.2.19) comes from the pole at $k = k_\omega$ and can be extracted by representing the cosine as a sum of two oscillating exponents. As a result, we get

$$G_\omega(R) \approx -\frac{im}{\sqrt{2\pi k_\omega R}}\, e^{i(k_\omega R - \pi/4)} \tag{3.2.22}$$

and, finally,

$$\delta\rho_\omega(R) = -\frac{m^2 V_0}{2\pi^2 k_\omega R} \cos(2k_\omega R)\,. \tag{3.2.23}$$

These Friedel oscillations have the same nature as those in the density correlations $\langle n(x)n(y)\rangle$ studied in Section 3.1.6, although the Green's functions are different in these two problems: equal-time ($t = 0$) vs. fixed-frequency).

Problem Set 6

Problem 6.1

(a) For a free particle in 3D, calculate the Green's functions $G_\omega(R)$ [in the frequency-coordinate representation, as defined in Eq. (3.2.4)]. In order to do this, calculate the three-dimensional version of the integral (3.2.18).

As in 2D, this Green's functions oscillates at the wave vector $k_\omega = \sqrt{2m\omega}$ and decays as a power of R. Compare this power with $R^{-1/2}$ for the 2D Green's function (3.2.22).

(b) If we study the effect discussed in Section 3.2.2 (density-of-states oscillations around an impurity) in 3D, then, at large R we would find

$$\delta\rho_\omega(R) \propto R^{-\alpha} \cos(2k_\omega R + \varphi) .$$

Find the power α.