

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:

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

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

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

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)

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

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

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

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:

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

where

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

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:

$$(H_0 + V)\Psi = E\Psi, \quad (3.2.7)$$

then we may formally solve it perturbatively by rewriting

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

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

$$G = \frac{1}{E - H_0 + i0} \quad (3.2.9)$$

The perturbative series for Ψ can be constructed iteratively

$$\Psi = \Psi_0 + \Psi_1 + \dots \quad (3.2.10)$$

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

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

As a result, we get the perturbative series

$$\Psi = (1 + GV + GVG V + \dots) \Psi_0, \quad (3.2.12)$$

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:

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

which is the operator counterpart of the usual power series:

$$\frac{1}{a - \epsilon} = \frac{1}{a} + \frac{1}{a^2} \epsilon + \frac{1}{a^3} \epsilon^2 + \dots \quad (3.2.14)$$

(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

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

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

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

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

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

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

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

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

$$G_\omega(R) = \int_0^\infty \frac{k J_0(kR)}{\omega - (k^2/2m) + i0} \frac{dk}{2\pi}, \quad (3.2.19)$$

where J_0 is the Bessel function:

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

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

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

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

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

and, finally,

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

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 .