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Green's function, LDOS and Friedel oscillations

In this tutorial we introduce the retarded Green's function and the local density of states. As an illustration we study Friedel oscillations for a simple one-dimensional model of non-interacting fermions.

1 Retarded Green's function in first quantization

Consider a first quantized Hamiltonian H, *e.g.*

$$H = \frac{p^2}{2m} + V(r)$$

and let $G_R(t,t')$ be an operator defined as

$$\begin{cases} (i\partial_t \mathbb{1} - H)\ G_R(t,t') = \delta(t-t')\mathbb{1}, \\ G_R(t,t') = 0 \ \text{ for } t < t' \end{cases} \tag{1}$$

We assume that H does not depend on time, and we set $\hbar = 1$.

1. Argue that G_R only depends on $t - t'$ and that the solution of the previous differential equation is:

$$\boxed{G_R(t,t') = -i\theta(t-t')e^{-iH(t-t')}} \tag{2}$$

Interpretation as a propagator

The operator $G_R(t,t')$ can be decomposed in real space: $G_R(r,t,r',t')$ is the (retarded) Green's function in real space and is given by:

$$\begin{cases} G_R(t,t') = \int dr\, dr'\, G_R(r,t,r',t')|r\rangle\langle r'|, \\ G_R(r,t,r',t') = \langle r|G_R(t,t')|r'\rangle \end{cases} \tag{3}$$

In mathematics, a Green's function is the impulse response of an inhomogeneous linear differential equation defined on a domain, with specified initial conditions or boundary conditions. The Schrödinger equation in real space is typically a differential equation

$$i\partial_t \Psi(r) = H(r)\Psi(r)$$

For instance if $H = \frac{p^2}{2m} + V(r)$, then the differential operator $H(r)$ is $H(r) = -\frac{\Delta}{2m} + V(r)$.

2. Check that

$$(i\partial_t \mathbb{1} - H(r))\ G_R(r,t,r',t') = \delta(t-t')\delta(r-r') \tag{4}$$

3. Consider the wavefunction at time t, $\Psi(r,t)$, obtained from the initial condition $\Psi(r,t') = \delta(r-r')$ (i.e. $|\Psi(t')\rangle = |r'\rangle$). Argue that $G_R(r,t,r',t')$ is the amplitude for a particle at time $t > t'$ to be measured at position r knowing that it was at position r' at time t'.

4. Check that, starting from an arbitrary initial state $\Psi(r',t')$ at time t', the state at time $t > t'$ is:

$$\Psi(r,t) = i \int dr' G_R(r,t,r',t')\Psi(r',t') \qquad \text{as long as } t > t' \tag{5}$$

Analytic properties of the (Fourier transform of) Green's function

5. Let $|\phi_\alpha\rangle$ be an eigenbasis of H, namely $H = \sum_\alpha \epsilon_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$. We have

$$G_R(r,t,r',t') = -i\theta(t-t') \sum_\alpha \phi_\alpha(r)\phi_\alpha^*(r')e^{-i\epsilon_\alpha(t-t')} \tag{6}$$

Let us define the time Fourier transform and its inverse:

$$\begin{cases} \tilde{G}_R(r,r',\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, G_R(r,t,r',0) \\ G_R(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\tilde{G}_R(\omega) \end{cases} \tag{7}$$

Show that, as long as ω is not in the spectrum of H, we can write

$$\tilde{G}_R(\omega) = (w\mathbb{1} - H)^{-1} = \sum_\alpha \frac{1}{\omega - \epsilon_\alpha}|\phi_\alpha\rangle\langle\phi_\alpha|, \qquad \omega \in \mathbb{C} \setminus \{\epsilon_\alpha, \alpha = 0,1,\cdots\} \tag{8}$$

This equation defines a meromorphic (analytic except for a discrete set of points) function of ω with simple poles at $w = \epsilon_\alpha$.
On the other hand since $(\omega - H)$ is not invertible for $w = \epsilon_\alpha$, the operator $(\omega - H)$ has infinitely many right inverses, and the equation $(\omega\mathbb{1} - H)\tilde{G}_R(\omega) = \mathbb{1}$ does not define $\tilde{G}_R(\omega)$ uniquely. To be more specific, once we have a particular solution $\tilde{G}^0_R(\omega)$, then a generic solution is of the form

$$\tilde{G}_R(\omega) = \tilde{G}^0_R(\omega) + \sum_{\alpha,\beta} a_{\alpha,\beta}\delta(\omega - \epsilon_\alpha)|\phi_\alpha\rangle\langle\phi_\beta| \tag{9}$$

In order to fix a unique solution, we must specify the behavior of $\tilde{G}_R(\omega)$ as $w \to \epsilon_\alpha$. The retarded Green's function amounts to the choice $G_R(t) = 0$ for negative t. This choice is motivated by causality, and it lifts any ambiguity from the definition of the Green's function. When performing the inverse Fourier transforms from $\tilde{G}_R(\omega)$, it amounts to avoiding the poles at $w = \epsilon_\alpha$ by integrating slightly above them in the complex plane[1]. This is typically written as

$$\boxed{\tilde{G}_R(\omega) = \lim_{\eta\to 0^+} (\omega + i\eta - H)^{-1} = (\omega + i0^+ - H)^{-1}} \tag{10}$$

However it is good to keep in mind that taking the limit $\eta \to 0$ is a rather subtle one[2].

[1] Indeed in that case the poles are $\epsilon_\alpha - i\eta$, i.e. in the lower half plane, and for $t < 0$ one can close the contour in the upper half plane, yielding $G_R(t) = 0$

[2] The relevant formula here being

$$\lim_{\eta\to 0^+} \int_0^\infty dt e^{it(\omega+i\eta)} = i \lim_{\eta\to 0^+} \frac{1}{\omega + i\eta} = i\mathcal{P}(1/\omega) + \pi\delta(\omega)$$

where $\mathcal{P}$ stands for Cauchy principal value.

2 Single-particle Green's functions in second quantization

The more generic definition of the retarded Green's function is

$$G_R(\alpha,t;\alpha',t') = -i\theta(t-t')\langle[c_\alpha(t), c^\dagger_{\alpha'}(t')]\rangle \qquad \text{for bosons} \tag{11}$$

$$= -i\theta(t-t')\langle\{c_\alpha(t), c^\dagger_{\alpha'}(t')\}\rangle \qquad \text{for fermions} \tag{12}$$

where α index the full one-body Hilbert space. For instance $\alpha = (\vec{r},\sigma)$ for spin-1/2 particles, in which case we have

$$G_R(r,\sigma,t';r'\sigma',t') = -i\theta(t-t')\langle[\Psi_\sigma(r,t), \Psi^\dagger_{\sigma'}(r',t')]_\pm\rangle \tag{13}$$

where $[\cdot,\cdot]_+$ is a commutator and $[\cdot,\cdot]_-$ an anti-commutator. We also have to specify what is meant by the mean value $\langle\cdots\rangle$. Several cases are possible

- for a closed system at zero temperature, $\langle X\rangle = \langle GS|X|GS\rangle$, where $|GS\rangle$ is the many-body ground state.
- for a closed system at inverse temperature β, we choose

  $$\langle X\rangle = Z^{-1}\mathrm{Tr}\left(Xe^{-\beta H}\right) = Z^{-1}\sum_n \langle\Psi_n|X|\Psi_n\rangle e^{-\beta E_n},$$

  where $|\Psi_n\rangle$ are the many-body eigenstates of the total Hamiltonian H, with energy E_n.

The zero temperature case is a special case and can be obtained by sending $\beta\to\infty$.

One can also define the so-called greater and lesser Green's functions, namely

$$G_>(\alpha,t;\alpha',t') = -i\langle c_\alpha(t)\, c^\dagger_{\alpha'}(t')\rangle \tag{14}$$

$$G_<(\alpha,t;\alpha',t') = \mp i\langle c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle \qquad \text{for bosons/ fermions} \tag{15}$$

so that

$$\boxed{G_R(\alpha,t;\alpha',t') = \theta(t-t')\left[G_>(\alpha,t;\alpha',t') - G_<(\alpha,t;\alpha',t')\right]} \tag{16}$$

6. Show that

$$\tilde{G}_<(\alpha,\alpha',\omega) = \pm e^{-\omega\beta}\tilde{G}_>(\alpha,\alpha',\omega) \tag{17}$$

7. Show that in the case of a non-interacting (*i.e.* quadratic) Hamiltonian

$$H = \sum_\alpha \epsilon_\alpha c^\dagger_\alpha c_\alpha \tag{18}$$

the many-body retarded Green's function coincides with the one defined in first quantization, namely

$$\tilde{G}_R(\alpha,\alpha',\omega) = \langle\alpha|\frac{1}{\omega+i0^+-h}|\alpha'\rangle \tag{19}$$

where $h = \sum_\alpha \epsilon_\alpha|\phi_\alpha\rangle\langle\phi_\alpha|$ is the corresponding one-body Hamiltonian.

The spectral function

We will now focus on the diagonal elements of the Green's function, and we define the **spectral function** as

$$\boxed{A(\alpha,\omega) = -2\,\mathrm{Im}\,\tilde{G}_R(\alpha,\alpha,\omega)} \tag{20}$$

8. Show that

$$A(\alpha,\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\,\langle [c_\alpha(t), c_\alpha^\dagger(0)]_\pm\rangle \tag{21}$$

and deduce

$$i\tilde{G}_>(\alpha,\alpha,\omega) = \frac{A(\alpha,\omega)}{1\mp e^{-\beta\omega}}, \tag{22}$$

$$\pm i\tilde{G}_<(\alpha,\alpha,\omega) = e^{-\beta\omega}\frac{A(\alpha,\omega)}{1\mp e^{-\beta\omega}} \tag{23}$$

9. Show that the spectral function $A(\alpha,\omega)$ behaves like a probability distribution of the variable ω :

$$A(\alpha,\omega)\geq 0, \qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,A(\alpha,\omega) = 1 \tag{24}$$

provided $\langle\alpha|\alpha\rangle = 1$ (for instance this does not work for the the real space LDOS in the continuum, since $|r\rangle$ is not normalizable.)

10. Argue that the mean occupation $\langle n_\alpha\rangle = \langle c_\alpha^\dagger c_\alpha\rangle$ is given by

$$\boxed{\langle n_\alpha\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-\beta\omega}}{1\mp e^{-\beta\omega}}A(\alpha,\omega)} \tag{25}$$

2.1 Density of states and local density of states (LDOS)

For a system of non-interacting particles (*i.e.* for an Hamiltonian of the form $H=\sum_n \epsilon_n c_n^\dagger c_n$) the density of states is defined as follow : $D(\epsilon)\Delta\epsilon$ is the number of one-particle states with an energy between ϵ and $\epsilon+\Delta\epsilon$. Typically it scales with the volume, so we are led to defined the density of states per volume $d(\epsilon) = D(\epsilon)/V$.

$$D(\epsilon) = \sum_n \delta(\epsilon-\epsilon_n) \tag{26}$$

11. Show that the density of states is equal to

$$\boxed{D(\epsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}\,G_R(\epsilon)} \tag{27}$$

A natural definition for the LDOS is

$$\rho(\alpha,\epsilon) = \sum_n |\langle\alpha|n\rangle|^2\delta(\epsilon-\epsilon_n) \tag{28}$$

whose interpretation is the following : $\rho(\alpha,\epsilon)\,\Delta\epsilon$ is the probability to find an electron in state $|\alpha\rangle$ and energy between ϵ and $\epsilon+\Delta\epsilon$.

12. Show that formula (28) is equivalent to

$$\boxed{\rho(\alpha,\omega) = \frac{1}{2\pi} A(\alpha,\omega) = -\frac{1}{\pi} \operatorname{Im} G_R(\alpha,\alpha,\omega)} \tag{29}$$

By extension the LDOS is defined for interacting systems by equation (29). In particular the spatially resolved density of state is

$$\rho(r,\omega) = -\frac{1}{\pi} \operatorname{Im} G_R(r,r,\omega) \tag{30}$$

3 Application: a simple one-dimensional model.

Consider a non-interacting, one-dimensional tight-binding model on N sites with periodic-boundary conditions.

$$H_0 = -t \sum_{j=1}^{N} \left(c_{j+1}^\dagger c_j + \text{h.c.} \right), \qquad c_{N+j} = c_j$$

As we have seen in the tutorial about the Hubbard model, such a quadratic model is straightforward to solve. We have

$$H_0 = \sum_k \epsilon_k \tilde{c}_k^\dagger \tilde{c}_k, \qquad \epsilon_k = -2t \cos k$$

where

$$\tilde{c}_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikj} c_j^\dagger, \qquad k = \frac{2\pi}{N} m, \quad m = 0, 1, \cdots, N-1$$

13. Compute the retarded Green's function $G_0(n,m,\omega)$.

14. We are interested in very large systems, so we take $N \to \infty$. The correct Fourier transform is now

$$\tilde{c}_k^\dagger = \sum_{j=-\infty}^{\infty} e^{ikj} c_j^\dagger, \qquad c_j^\dagger = \int_0^{2\pi} \frac{dk}{2\pi} e^{-ikj} \tilde{c}_k^\dagger$$

Argue that the retarded Green's function is

$$\boxed{G_0(n,m,\omega) = \int_0^{2\pi} \frac{dk}{2\pi} \frac{e^{ik(n-m)}}{\omega + i0^+ - \epsilon_k}}$$

15. * Using the residue theorem, show that $G_0(n,m,\omega)$ is given by

$$G_0(n,m,\omega = -2t\cos\theta) = \frac{e^{i|n-m|\theta}}{2it\sin\theta}, \qquad \text{for} \qquad -2t < \omega < 2t \quad (0 < \theta < \pi)$$
$$G_0(n,m,\omega = 2t\cosh\theta) = \frac{(-1)^{n-m} e^{-|n-m|\theta}}{2t\sinh\theta}, \qquad \text{for} \qquad \omega > 2t \quad (\theta > 0)$$
$$G_0(n,m,\omega = -2t\cosh\theta) = -\frac{e^{-|n-m|\theta}}{2t\sinh\theta}, \qquad \text{for} \qquad \omega < -2t \quad (\theta > 0)$$

while $G_0(n,m,\omega)$ diverges for $\omega = \pm 2t$ (why could that be expected ?).

16. Compute the density of states (per unit volume *i.e.* per site) directly from the spectrum. Recover this result using the Green's function.

17. We add an impurity at position 0

$$H = H_0 + V, \qquad V = v c_0^\dagger c_0$$

Show that

$$G = (1 - G_0 V)^{-1} G_0 = G_0 + G_0 T(\omega) G_0, \qquad T(\omega) = V + V G_0(\omega) V + V G_0(\omega) V G_0(\omega) V + \cdots \quad (31)$$

18. Show that $T(\omega) = \frac{v}{1 - v G_0(0,0,\omega)} |0\rangle\langle 0|$.

19. Let $\delta\rho(n,\omega) = \rho(n,\omega) - \rho_0(n,\omega)$ be the variation of the LDOS due to the impurity. Compute $\delta\rho(n,\omega)$ at zero temperature and half-filling for ω close to the Fermi energy.