Chapter 4

The single–particle Green's function

Green's functions are very useful for solving certain partial differential equations, for instance the inhomogeneous wave equations in electrodynamics (see J.D. Jackson, Classical Electrodynamics,

Section 6.6). In many-body physics a generalized version of Green's functions turns out not only to be extremely helpful for analysing certain problems, but also to contain itself a wealth of information about the dynamics of the many-particle system. In this chapter we limit ourselves on the single-particle Green's function; two-particle Green's functions, which are related to various response functions or susceptibilities, will not be considered. Furthermore, we consider only Green's functions at zero temperature. Green's functions at finite temperatures, especially the so-called Matsubara Green's functions, do not present additional complications. Essentially, the ground state expectation values are replaced by averages with respect to the grand-canonical ensemble.

4.1 Basic Definitions

We consider a many-body system described by a Hamiltonian H, for instance a system of fermions or bosons with short-range interactions. In the Heisenberg picture the time-evolution is given by the time-dependence of creation and annihilation operators

$$\begin{aligned} \Psi_\sigma(\mathbf{r},t) &= e^{\frac{i}{\hbar}Ht}\,\Psi_\sigma(\mathbf{r})e^{-\frac{i}{\hbar}Ht}\,, \\ a_{\mathbf{k}\sigma}(t) &= e^{\frac{i}{\hbar}Ht}\,a_{\mathbf{k}\sigma}e^{-\frac{i}{\hbar}Ht}\,. \end{aligned} \tag{4.1}$$

We define the time-ordering symbol T as an operator which orders a product of time-dependent operators in such a way that the early times are to the right and later times to the left, *i.e.*

$$T\left[\Psi_\sigma(\mathbf{r}_1,t_1)\ \Psi^\dagger_\sigma(\mathbf{r}_2,t_2)\right] = \begin{cases} \Psi_\sigma(\mathbf{r}_1,t_1)\,\Psi^\dagger_\sigma(\mathbf{r}_2,t_2), & t_1 > t_2\,, \\ \pm\Psi^\dagger_\sigma(\mathbf{r}_2,t_2)\ \Psi_\sigma(\mathbf{r}_1,t_1)\,, & t_1 < t_2\,, \end{cases} \tag{4.2}$$

where the plus and minus signs stand for bosons and fermions, respectively. Let $|\Psi_0>$ describe the exact ground state of N particles. The single-particle Green's function is then defined as

$$G_\sigma(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -i\left\langle \Psi_0 \left| T\left[\Psi_\sigma(\mathbf{r}_1,t_1)\,\Psi_\sigma^\dagger(\mathbf{r}_2,t_2)\right]\right| \Psi_0\right\rangle . \tag{4.3}$$

Here we have implicitly assumed that there are no spin-dependent interactions (such as spin-orbit interactions which would require matrix Green's functions $G_{\sigma_1\sigma_2}$). If the Hamiltonian is time-independent, the Green's function depends only on $t := t_1 - t_2$. Moreover, if the system is translationally invariant, G depends only on $\mathbf{r} := \mathbf{r}_1 - \mathbf{r}_2$ (this is not true for electrons in a periodic lattice potential). In this case we can introduce the Fourier transform,

$$G_\sigma(\mathbf{r}_1 t_1;\mathbf{r}_2,t_2) = G_\sigma(\mathbf{r},t) = \int \frac{d\omega}{2\pi}\int \frac{d^3k}{(2\pi)^3}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}G_\sigma(\mathbf{k},\omega)\,,$$

$$G_\sigma(\mathbf{k},\omega) = \int dt \int d^3r\; e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\,G_\sigma(\mathbf{r},t)\,. \tag{4.4}$$

In view of Eq. (2.26) it is easy to see that $G_\sigma(\mathbf{k},\omega)$ is the (time) Fourier transform of

$$G_\sigma(\mathbf{k},t) = -i\left\langle \Psi_0 | T\left[a_{\mathbf{k}\sigma}\,(t) a_{\mathbf{k}\sigma}^\dagger\right]|\Psi_0\right\rangle . \tag{4.5}$$

The Green's function (4.3) can be interpreted as follows. Let us consider the case $t_1 > t_2$ first where

$$G_\sigma(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -i\left\langle \Psi_0|e^{\frac{i}{\hbar}Ht_1}\Psi_\sigma(\mathbf{r}_1)\,e^{-\frac{i}{\hbar}H(t_1-t_2)}\Psi_\sigma^+(\mathbf{r}_2)\,e^{-\frac{i}{\hbar}Ht_2}|\Psi_0\right\rangle .$$

We first let evolve the exact ground state until the time t_2 where we add a particle at $\mathbf{r}_2$, then the system evolves further during the time interval $t_1 - t_2$. The scalar product between the resulting state and a state where at time t_1 a particle has been added at $\mathbf{r}_1$ is then given by the Green's function. Similarly for $t_1 < t_2$ we seek the overlap between a state obtained by removing at time t_1 a particle at $\mathbf{r}_1$, with a subsequent evolution until t_2, and a state where at time t_2 a particle is removed at $\mathbf{r}_2$.

More important than this interpretation is the use of the single-particle Green's function for calculating observable quantities. Thus the occupation number of the single-particle state $\mathbf{k}\sigma$ is

$$\langle \Psi_0 \left| a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}\right| \Psi_0\rangle = \pm i \lim_{t\uparrow 0} G_\sigma(\mathbf{k},t)\,. \tag{4.6}$$

4.2 Free fermions

We consider the simple case of free bosons or fermions in a box of volume V. The Hamiltonian is given by Eq. (2.30),

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_k\, a_{\mathbf{k}\sigma}^\dagger\, a_{\mathbf{k}\sigma}\,, \tag{4.7}$$

with a single-particle spectrum $\varepsilon_k = \frac{(\hbar k)^2}{2m}$. For this case the time dependence is given by

$$a_{\mathbf{k}\sigma}(t) = e^{\frac{i}{\hbar}\varepsilon_k t\, a_{\mathbf{k}\sigma}^\dagger\, a_{\mathbf{k}\sigma}}\; a_{\mathbf{k}\sigma} e^{-\frac{i}{\hbar}\varepsilon_k t\, a_{\mathbf{k}\sigma}^\dagger\, a_{\mathbf{k}\sigma}}\,.$$

This operator satisfies the differential equation

$$\frac{d}{dt}a_{\mathbf{k}\sigma}(t) = \frac{i}{\hbar}\varepsilon_k \left[a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma},\, a_{\mathbf{k}\sigma}\right](t) = -\frac{i}{\hbar}\varepsilon_k\, a_{\mathbf{k}\sigma}(t)\,,$$

with the initial condition

$$a_{\mathbf{k}\sigma}(0) = a_{\mathbf{k}\sigma}\,.$$

Its solution is

$$a_{\mathbf{k}\sigma}(t) = e^{-\frac{i}{\hbar}\varepsilon_k t}\, a_{\mathbf{k}\sigma}\,. \tag{4.8}$$

This expression can also be easily obtained by acting with $a_{\mathbf{k}\sigma}(t)$ on a general basis state in occupation number representation.

We use now this result for calculating the free fermion Green's function, where in the ground state all levels $\mathbf{k}\sigma$ are occupied up to the Fermi energy ε_F and empty above,

$$\langle\Psi_0\left|a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}\right|\Psi_0\rangle =: f_{\mathbf{k}\sigma} = \begin{cases} 1 & , \quad \varepsilon_k < \varepsilon_F, \\ 0 & , \quad \varepsilon_k > \varepsilon_F\,. \end{cases} \tag{4.9}$$

Inserting Eq. (4.8) into Eq. (4.5) we obtain

$$G_\sigma(\mathbf{k},t) = -i\left[\vartheta(t)\,(1-f_{\mathbf{k}\sigma}) - \vartheta(-t)\, f_{\mathbf{k}\sigma}\right] e^{-\frac{i}{\hbar}\varepsilon_k t}\,, \tag{4.10}$$

where $\vartheta(t)$ is the step function

$$\vartheta(t) = \begin{cases} 1 & , \quad t>0\,, \\ 0 & , \quad t<0\,. \end{cases} \tag{4.11}$$

One immediately verifies that Eq. (4.10) agrees with Eq. (4.6). The Green's function (4.10) satisfies the differential equation

$$\left(i\frac{\partial}{\partial t} - \frac{\varepsilon_k}{\hbar}\right) G_\sigma(\mathbf{k},t) = \delta(t)\,. \tag{4.12}$$

Therefore $G_\sigma(\mathbf{k},t)$ is indeed a Green's function in the sense of the quantity introduced for solving differential equations; it is the Green's function of the operator $i\frac{\partial}{\partial t} - \frac{\varepsilon_k}{\hbar}$.

The Fourier transform of Eq. (4.10) is ill-defined because of the oscillatory behavior for $t \to \pm\infty$. Therefore we consider the function

$$e^{-\eta|t|}\, G_\sigma(\mathbf{k},t), \quad \text{where} \quad \eta > 0\,.$$

Its Fourier transform is

$$\int dt\, e^{i\omega t}\, e^{-\eta|t|}\, G_\sigma(\mathbf{k},t) = \frac{1-f_{\mathbf{k}\sigma}}{\omega - \frac{\varepsilon_k}{\hbar} + i\eta} + \frac{f_{\mathbf{k}\sigma}}{\omega - \frac{\varepsilon_k}{\hbar} - i\eta}\,. \tag{4.13}$$

We use the notation $G_\sigma(\mathbf{k},\omega)$ for this expression in the limit where η is infinitesimal. Together with the definition

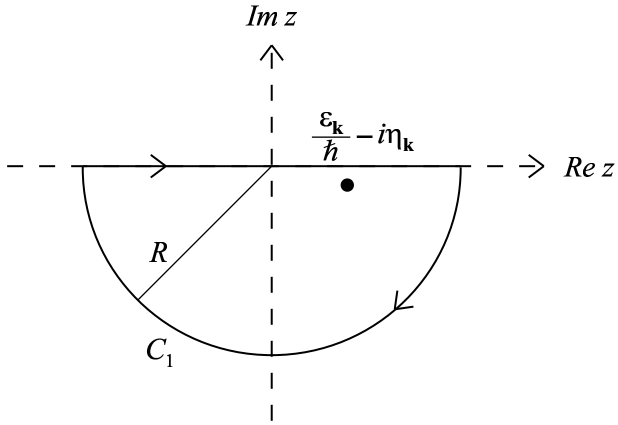
$$\eta_k := \eta \quad \operatorname{sign}(\varepsilon_k - \varepsilon_F) \tag{4.14}$$

we obtain the simple result

$$G_\sigma\left(\mathbf{k},\omega\right)=\frac{1}{\omega-\frac{\varepsilon_k}{\hbar}+i\eta_k}\,. \tag{4.15}$$

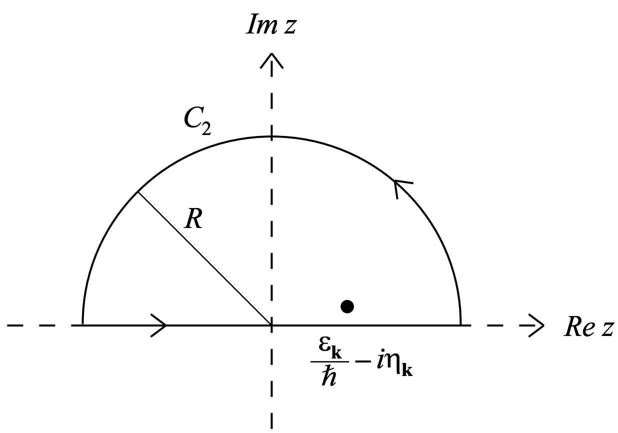
For the inverse transform we integrate along contours in the complex plane. For $t>0$ we have to integrate in the lower half-plane where the contribution over the semi-circle vanishes for $R\to\infty$:

$$\begin{aligned}\int\frac{d\omega}{2\pi}e^{-i\omega t}\frac{1}{\omega-\frac{\varepsilon_k}{\hbar}+i\eta_k} &= \lim_{R\to\infty}\int_{C_1}\frac{dz}{2\pi}e^{-izt}\frac{1}{z-\frac{\varepsilon_k}{\hbar}+i\eta_k}\\ &= -i\,e^{-\frac{i}{\hbar}\varepsilon_k t}e^{-\eta t}\,\vartheta(\varepsilon_k-\varepsilon_F)\,. \end{aligned}\tag{4.16}$$



For $t<0$ we integrate in the upper half-plane and obtain:

$$\begin{aligned}\int\frac{d\omega}{2\pi}e^{-i\omega t}\frac{1}{\omega-\frac{\varepsilon_k}{\hbar}+i\eta_k} &= \lim_{R\to\infty}\int_{C_2}\frac{dz}{2\pi}e^{-izt}\frac{1}{z-\frac{\varepsilon_k}{\hbar}+i\eta_k}\\ &= ie^{-\frac{i}{\hbar}\varepsilon_k t}\,e^{\eta t}\,\vartheta(\varepsilon_F-\varepsilon_k)\,. \end{aligned}\tag{4.17}$$



The comparison of Eqs. (4.16) and (4.17) with Eq. (4.10) yields

$$\int\frac{d\omega}{2\pi}\,e^{-i\omega t}G_\sigma(\mathbf{k},\omega)=e^{-\eta|t|}G_\sigma(\mathbf{k},t)\,, \tag{4.18}$$

as expected.

4.3 Spectral representation

We turn now to an interacting many-fermion system with translational symmetry and spin-independent forces between the particles and thus consider the Green's function (4.5). Using the completeness relation in Fock space

$$\mathbf{1} = |0\rangle\langle 0| + \sum_n |\Psi_n^{(1)}\rangle\langle\Psi_n^{(1)}| + \sum_n |\Psi_n^{(2)}\rangle\langle\Psi_n^{(2)}| + \ldots,$$

where $|0\rangle$ is the vacuum state and $|\Psi_n^{(i)}\rangle$ is the n'th eigenstate of the Hamiltonian with i particles, we can write the Green's function as

$$\begin{aligned} G_\sigma(\mathbf{k},t) &= -i\Big\{\vartheta(t)\sum_n \langle\Psi_0|a_{\mathbf{k}\sigma}(t)|\Psi_n^{(N+1)}\rangle\langle\Psi_n^{(N+1)}|a^\dagger_{\mathbf{k}\sigma}|\Psi_0\rangle \\ &\quad -\vartheta(-t)\sum_n < \Psi_0|a^\dagger_{\mathbf{k}\sigma}|\Psi_n^{(N-1)}\rangle\langle\Psi_n^{(N-1)}|a_{\mathbf{k}\sigma}(t)|\Psi_0\rangle\Big\}\,, \end{aligned}$$

where $|\Psi_0\rangle$ is the N-particle ground state. The relations

$$\begin{aligned} \langle\Psi_0|a_{\mathbf{k}\sigma}(t)|\Psi_n^{(N+1)}\rangle &= e^{\frac{i}{\hbar}(E_0^{(N)}-E_n^{(N+1)})t}\langle\Psi_0|a_{\mathbf{k}\sigma}|\Psi_n^{(N+1)}\rangle\,, \\ \langle\Psi_n^{(N-1)}|a_{\mathbf{k}\sigma}(t)|\Psi_0\rangle &= e^{\frac{i}{\hbar}(E_n^{(N-1)}-E_0^{(N)})t}\langle\psi_n^{(N-1)}|a_{\mathbf{k}\sigma}|\Psi_0\rangle \end{aligned}$$

allow us to calculate explicitly the Fourier transform of $G_\sigma(\mathbf{k},t)e^{-\eta|t|}$,

$$\begin{aligned} G_\sigma(\mathbf{k},\omega) &= -i\sum_n\int_0^\infty dt\, e^{i\left[\omega+i\eta+\frac{E_0^{(N)}-E_n^{(N+1)}}{\hbar}\right]t}\left|\langle\Psi_n^{(N+1)}|a^\dagger_{\mathbf{k}\sigma}|\Psi_0\rangle\right|^2 \\ &\quad +i\sum_n\int_{-\infty}^0 dt\, e^{i\left[\omega-i\eta+\frac{E_n^{(N-1)}-E_0^{(N)}}{\hbar}\right]t}\left|\langle\Psi_n^{(N-1)}|a_{\mathbf{k}\sigma}|\Psi_0\rangle\right|^2 \\ &= \sum_n\left\{\frac{\left|\langle\Psi_n^{(N+1)}|a^\dagger_{\mathbf{k}\sigma}|\Psi_0\rangle\right|^2}{\omega+\frac{E_0^{(N)}-E_n^{(N+1)}}{\hbar}+i\eta}+\frac{\left|\langle\Psi_n^{(N-1)}|a_{\mathbf{k}\sigma}|\Psi_0\rangle\right|^2}{\omega+\frac{E_n^{(N-1)}-E_0^{(N)}}{\hbar}-i\eta}\right\}. \qquad (4.19) \end{aligned}$$

The operator $a^\dagger_{\mathbf{k}\sigma}$ in the first term increases the momentum by $\hbar\mathbf{k}$ and the energy by

$$E_n^{(N+1)} - E_0^{(N)} = \varepsilon_n^{(N+1)} + \mu_N$$

where $\varepsilon_n^{(N+1)} := E_n^{(N+1)} - E_0^{(N+1)}$ is the excitation energy and $\mu_N := E_0^{(N+1)} - E_0^{(N)}$ is the chemical potential. Correspondingly, the operator $a_{\mathbf{k}\sigma}$ in the second term removes a momentum $\hbar\mathbf{k}$ and an energy

$$E_0^{(N)} - E_n^{(N-1)} = \mu_{N-1} - \varepsilon_n^{(N-1)}\,.$$

We assume that the differences between the chemical potentials μ_N and μ_{N-1} and between the excitation energies $\varepsilon_n^{(N\pm1)}$ are of order $\frac{1}{N}$ and can be neglected. (There are cases where this is not always true, for instance a semiconductor with an energy gap between valence and conduction band.) We define the spectral densities $A(\mathbf{k},\omega)$ and $B(\mathbf{k},\omega)$ by the relations

$$\begin{aligned} A(\mathbf{k},\omega) &:= \sum_n \left|\langle\Psi_n^{(N+1)}|a_{\mathbf{k}\sigma}^\dagger|\Psi_0\rangle\right|^2 \delta\left(\omega - \frac{\varepsilon_n}{\hbar}\right), \\ B(\mathbf{k},\omega) &:= \sum_n \left|\langle\Psi_n^{(N-1)}|a_{\mathbf{k}\sigma}|\Psi_0\rangle\right|^2 \delta\left(\omega - \frac{\varepsilon_n}{\hbar}\right). \end{aligned} \tag{4.20}$$

Both functions vanish for $\omega < 0$ and we can write $G_\sigma(\mathbf{k},\omega)$ as an integral

$$G_\sigma(\mathbf{k},\omega) = \int_0^\infty d\omega' \left\{\frac{A(\mathbf{k},\omega')}{\omega-\omega'-\frac{\mu}{\hbar}+i\eta} + \frac{B(\mathbf{k},\omega')}{\omega+\omega'-\frac{\mu}{\hbar}-i\eta}\right\}. \tag{4.21}$$

In the large volume limit the excitation energies ε_n are expected to be dense so that the spectral densities become smooth (real and positive) functions of ω. Then the integration in Eq. (4.21) can be separated into real and imaginary parts,

$$ReG_\sigma(\mathbf{k},\omega) = ⨍_0^\infty d\omega' \left\{\frac{A(\mathbf{k},\omega')}{\omega-\omega'-\frac{\mu}{\hbar}} + \frac{B(\mathbf{k},\omega')}{\omega+\omega'-\frac{\mu}{\hbar}}\right\}, \tag{4.22}$$

$$ImG_\sigma(\mathbf{k},\omega) = \begin{cases} -\pi A(\mathbf{k},\omega-\frac{\mu}{\hbar}) & , \quad \omega > \frac{\mu}{\hbar}, \\ \pi B(\mathbf{k},-\omega+\frac{\mu}{\hbar}) & , \quad \omega < \frac{\mu}{\hbar}. \end{cases} \tag{4.23}$$

Here $⨍$ indicates the principal part

$$⨍_{x_1}^{x_2} dx\, \frac{f(x)}{x-x_0} = \lim_{\varepsilon\to 0}\left\{\int_{x_1}^{x_0-\varepsilon} dx\, \frac{f(x)}{x-x_0} + \int_{x_0+\varepsilon}^{x_2} dx\, \frac{f(x)}{x-x_0}\right\},$$

if $x_1 < x_0 < x_2$, and the imaginary part comes from the semi-circles around the simple poles. Sometimes one writes symbolically

$$\lim_{\eta\to 0^\dagger} \frac{1}{x-x_0 \pm i\eta} = P\frac{1}{x-x_0} \mp i\pi\,\delta(x-x_0). \tag{4.24}$$

Eq. (4.23) implies that the imaginary part of $G(\mathbf{k},\omega)$ changes sign for $\omega = \mu/\hbar$. Inserting Eq. (4.23) into (4.22) we obtain the dispersion relation

$$\begin{aligned} ReG_\sigma(\mathbf{k},\omega) &= \frac{1}{\pi}⨍_0^\infty d\omega' \left\{-\frac{ImG_\sigma(\mathbf{k},\omega'+\frac{\mu}{\hbar})}{\omega-\omega'-\frac{\mu}{\hbar}} + \frac{ImG_\sigma(\mathbf{k},-\omega'+\frac{\mu}{\hbar})}{\omega+\omega'-\frac{\mu}{\hbar}}\right\} \\ &= \frac{1}{\pi}⨍_{-\infty}^\infty d\omega' \frac{ImG_\sigma(\mathbf{k},\omega')}{\omega'-\omega}\,\mathrm{sign}\,(\omega'-\mu/\hbar). \end{aligned} \tag{4.25}$$

4.4 Quasi-particle poles

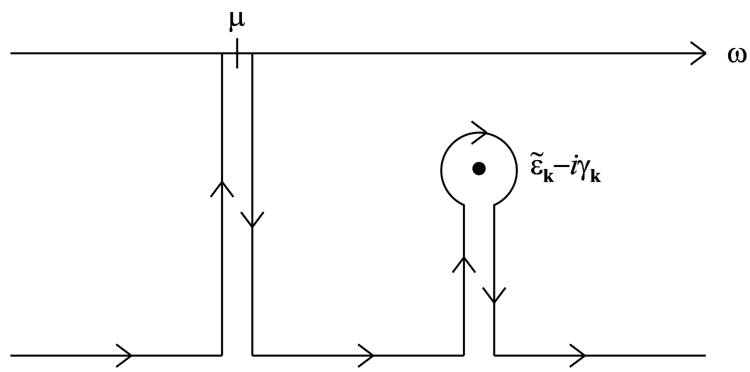
For independent fermions the Green's function $G_\sigma(\mathbf{k},t)$ is given by Eq. (4.10), *i.e.*, for $t > 0$

$$G_\sigma(\mathbf{k},t) = -i\vartheta(\varepsilon_k-\mu)e^{-\frac{i}{\hbar}\varepsilon_k t}. \tag{4.26}$$

$G_\sigma(\mathbf{k},\omega)$ has a simple pole at $\frac{\varepsilon_k}{\hbar} - i\eta$ for $\varepsilon_k > \mu$ (cf. Eq. (4.15)). We now discuss the Green's function for interacting fermions

$$G_\sigma(\mathbf{k},t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G_\sigma(\mathbf{k},\omega)\,.$$

For $\omega < \mu$ $G_\sigma(\mathbf{k},\omega)$ is equal to $G_A(\mathbf{k},\omega)$; therefore it is analytic in the lower half-plane. For $\omega > \mu$ $G_\sigma(\mathbf{k},\omega)$ is equal to $G_R(\mathbf{k},\omega)$, which is expected to have singularities in the lower half-plane. We assume that there is a simple pole at $\tilde{\varepsilon}_k - i\gamma_k$. We can then deform the integration contour as follows:



Here G_σ is replaced by G_A to the left of $\omega = \mu$ and by G_R at the right-hand side. The integral over the horizontal line is very small if t is sufficiently large. One can also show that the integrals over γ_1 and γ_2 can be neglected if $\frac{\hbar}{\tilde{\varepsilon}_k - \mu} \ll t \ll \frac{\hbar}{\gamma_k}$ (see Abrikosov et al., Section 7.2). This is only possible if $\gamma_k \ll (\tilde{\varepsilon}_k - \mu)$. In this case the only contribution arises from the circle surrounding the pole, i.e.

$$G_\sigma(\mathbf{k},t) \approx -ia\; e^{-\frac{i}{\hbar}\tilde{\varepsilon}_k t}\; e^{-\frac{1}{\hbar}\gamma_k t}\,, \tag{4.27}$$

where a is the residue of G_R at the pole. Thus the time dependence (4.26), which is just that of a single particle, is replaced by that of a quasi-particle with a renormalized energy $\tilde{\varepsilon}_k$ and a finite lifetime $\frac{\hbar}{\gamma_k}$. Due to the Pauli principle scattering processes close to the Fermi surface are strongly reduced so that the inequality $\gamma_k \ll (\tilde{\varepsilon}_k - \mu)$ appears to be very reasonable in this region. On the other hand the assumption of a simple pole is not always justified. In one dimension branch cuts can occur instead.

Literature

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