IV. THE PHYSICAL CONTENT OF THE GREEN'S FUNCTION

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A. Finite-temperature Green's function

The last time we have derived some rules for the perturbative calculation of the total energy of a many-body system. We have further seen, that the perturbative structure may be easier discussed in terms of the one-particle Green's function

$$\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2;\tau) = \begin{cases} -\mathrm{Tr}\left[e^{-(\beta-\tau)(H-\mu N)}\Psi(\mathbf{r}_1)e^{-\tau(H-\mu N)}\Psi^\dagger(\mathbf{r}_2)\right], & \text{for } \tau>0 \\ \mp\mathrm{Tr}\left[e^{-(\beta+\tau)(H-\mu N)}\Psi^\dagger(\mathbf{r}_2)e^{\tau(H-\mu N)}\Psi(\mathbf{r}_1)\right], & \text{for } \tau<0 \end{cases} \tag{1}$$

The connection to the non-interacting Green's function G_0 is given by Dyson's equation for the inverse of the operators

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma \tag{2}$$

and perturbation theory is directly formulated to calculate the selfenergy Σ. Dyson's equation, Eq. (2), is a matrix notation in the space-time representation, but for a homogeneous system, The equation simplifies if we chose the diagonal representation using Fourier space and Matsubara frequencies.

$$\begin{aligned} \mathcal{G}(\mathbf{r}) &= \mathcal{G}(\mathbf{r}_1,\mathbf{r}_1+\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{r}}\mathcal{G}(\mathbf{p}) \\ \mathcal{G}(\mathbf{p}) &= \int d\mathbf{r} e^{-i\mathbf{p}\cdot\mathbf{r}}\mathcal{G}(\mathbf{r}) \end{aligned} \tag{3}$$

The equivalent of the Fourier-transform in energy-time space is given by the representation using Matsubara frequencies

$$\mathcal{G}(\omega_n) = \int_0^\beta e^{i\omega_n\tau}\mathcal{G}(\tau)d\tau \tag{4}$$

where

$$\omega_n = 2n\pi T, \quad \text{for bosons} \tag{5}$$

$$\omega_n = (2n+1)\pi T, \quad \text{for fermions} \tag{6}$$

are the Matsubara frequency with $n = 0, \pm1, \pm2, \ldots$.

The non-interacting Green's function writes

$$\mathcal{G}_0^{-1}(\mathbf{p},\omega_n) = [i\omega_n + \mu - \varepsilon_p] \tag{7}$$

Feynman's rules in momentum/ frequency space are rather simple, since the interaction vertex conserves the total momentum/ energy, so that the sum of all in-coming momenta/ Matsubara-frequencies must equal the sum of all out-coming momenta/ Matsubara-frequencies.

B. Hartree-Fock, T-matrix, RPA

There are certain classes of diagrams which can be summed up easily. We will see that it is quite often neccessary to treat the diagrams inside these classes consistently in order to obtain a better behaved perturbation expansion in

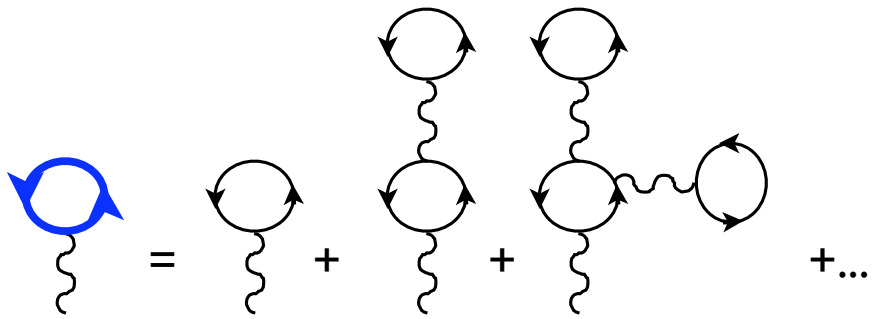

FIG. 1: The direct term of the self-energy in the Hartree-Fock approximation and its expansion in bare propagators.

renormalized parameter space. In the folllowing we will consider Bose systems, however, most of the analysis can be extended to Fermions.

Hartree-Fock. The mean-field Hartree-Fock equations are obtained by the following approximation for the self-energy

$$\Sigma_{HF}(\mathbf{k}) = -T\sum_{n'}\int \frac{d\mathbf{p}}{(2\pi)^3}\left[v(0)\mathcal{G}_{HF}(p,\omega_n') + v(|\mathbf{p}-\mathbf{k}|)\mathcal{G}_{HF}(p,\omega_n')\right] \tag{8}$$

where $\mathcal{G}_{HF}$ is the full propagator within this approximation

$$\mathcal{G}_{HF}^{-1} = G_0^{-1} - \Sigma_{HF} \tag{9}$$

Note that the self-energy is independant of ω_n in this approximation. Let us for the moment consider a system where the interaction potential is sufficiently weak, and does not depend on momentum (at least in the energy-region considered), $v(p) \simeq v(0) \equiv g$. In that case the self-energy is also momentum independant and is proportional to the density

$$\Sigma_{HF} = 2gn_{HF} \tag{10}$$

$$n_{HF} = -T\sum_{n}\int \frac{d\mathbf{p}}{(2\pi)^3}\mathcal{G}_{HF}(p,\omega_n) \tag{11}$$

$$= \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{1}{e^{\beta(\varepsilon_p+\Sigma_{HF}-\mu)}-1} \tag{12}$$

$$= \lambda^{-3} g_{3/2}\left(e^{\beta(\mu-\Sigma_{HF})}\right) \tag{13}$$

Bose-Einstein condensation is reached in this approximation when $\mu = \Sigma_{HF}$, which is a selfconsistent equation for μ. Let us approach the phase transition, setting $\Sigma_{HF} - \mu \to 0^+$. We have $g_{3/2}(e^x) \simeq 2.61 - 3.54\sqrt{-x}$, $n_{HF} \sim \mathcal{O}(1)$, and therefore $\Sigma_{HF} \sim \mathcal{O}(g)$ is linear in the coupling constant of the interaction. However, due to the non-analytic behavior of the $g_{3/2}$, the region of validity of any Taylor expansion around $\Sigma_{HF} - \mu = 0$ is zero.

What do we get if we would have started with the strict (not self-consistent) perturbation expansion? The first and second order terms included by the Hartree-Fock analyis are

$$\Sigma_{HF}^{(2)} = -2g\sum_{n}\int \frac{d\mathbf{p}}{(2\pi)^3}\mathcal{G}_0(\mathbf{p},n)\left\{1 - gT\sum_{n'}\int \frac{d\mathbf{p}'}{(2\pi)^3}[\mathcal{G}_0(\mathbf{p}',n')]^2\right\} \tag{14}$$

Now the second term inside the bracket on the rhs behaves roughly like the derivative of the bare density with respect to μ, and we see that the mean-field actually contains a summation of a series in $g/|\beta\mu|^{1/2}$. If we want to approach the point of $|\mu| \to 0$ higher orders in the perturbation theory diverge even more strongly. In our case, these problems occur do to so-called "infrared divergencies": in the limit of $\mu \to 0$, $\mathcal{G}(k,0) \sim \mu - k^{-2}/2m$ The Green's function approach allows us to estimate by simple dimensional analysis the effect of these infrared divergencies looking at the stricture of the integrals. We can see that he simple Hartree-Fock resummation cures the most diverging part,

however, as soon as $\beta(\mu-\Sigma)\sim g^2$ additional diagrams have to be considered. Therefore, mean-field can be trusted outside this "critical region".

Infrared problems are typical for phase-transitions, the renormalization group methods have developped powerful tools to "control" these problems. However, they all rely on basic assumptions of the (perturbative) analytic structure of the propagators.

T-matrix. A different series which can be treated and which is potentially divergent for short range potentials (particularly hard-core), is related to the two-particle scattering problem. Let us consider particle-particle scattering. In terms of Green's function this is most easily done in terms of the two-particle Green's function $\mathcal{G}_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2';\tau)$, defined as the average over two annihilation and two creation operators. Repeated particle-particle scattering can be written as a self-consistent equation for $\mathcal{G}_2$ in a matrix notation (numbers occuring twice are integrated over)

$$\mathcal{G}_2(1,2;1',2') \;=\; \mathcal{G}(1,1')\mathcal{G}(2,2')+\mathcal{G}(1,2';\tau)\mathcal{G}(2,1')+\mathcal{G}(1,\bar{1})\mathcal{G}(2,\bar{2},4)V(\bar{1},\bar{2})\mathcal{G}_2(\bar{1},\bar{2};1',2') \tag{15}$$

In the limit of $\beta\mu\to-\infty$ the system is dilute and the equation will include only two-particles scattering which each other. The two-body problem is solved by the complex T-matrix. For a dilute system G_2 can be replaced by the twi-body T-matrix which includes already repeated particle-particle scattering events. The on-shell T-matrix can be expressed in terms of the phase shifts, and in particular at low energies it reduces to a constant $4\pi\hbar^2a/m$ where a is the scattering length.

RPA-approximation. The so-called RPA-approximation introduces another class of diagrams which are conviniently expressed by an effective interaction V_{eff} which includes the effect of repeated density-fluctuations

$$V_{eff}(1,2;1',2')=v(1-2)+v(1-2)\mathcal{G}(1,\bar{1})\mathcal{G}(2,\bar{2})v_{eff}(\bar{1},\bar{2};1',2') \tag{16}$$

The corresponding diagrams are particularily important for long-range (Coulomb) interactions where they lead to an effective screened potential. A rearrangement of the perturbation theory in terms of the effective screened potential is possible and gives finite results in the dilute limit, for example in the electron-gas.

C. Analytic properties

Lehmann representation. Let us analyse the single particle Green's function, Eq. (1), using exact energy eigenstates, $|E_n^N\rangle$, of the N-particle system, $H|E_n^N\rangle=E_n|E_n^N\rangle$. We get

$$\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2;\tau)=\begin{cases}-\frac{1}{Z}\sum_n e^{-(\beta-\tau)(E_n^N-\mu N)}\langle E_n^N|\Psi(\mathbf{r}_1 0)|E_m^{N+1}\rangle\langle E_m^{N+1}|\Psi^\dagger(\mathbf{r}_2,0)|E_n^N\rangle e^{-\tau(E_m^{N+1}-\mu(N+1))}, & \text{for } \tau>0\\ \mp\frac{1}{Z}\sum_n e^{-(\beta-\tau)(E_n^N-\mu N)}\langle E_n^N|\Psi^\dagger(\mathbf{r}_1,0)|E_m^{N-1}\rangle\langle E_m^{N-1}|\Psi(\mathbf{r}_2,0)|E_n^N\rangle e^{-\tau(E_m^{N-1}-\mu(N-1))}, & \text{for } \tau<0\end{cases} \tag{17}$$

or, in Fourier space and Matsubara frequencies

$$\mathcal{G}(\mathbf{p};i\omega_k)=-\int_0^\beta d\tau\frac{1}{Z}\sum_{N,n,m}e^{-\beta(E_n^N-\mu N)}e^{(i\omega_k+E_n^N-E_m^{N+1}+\mu)\tau}\langle E_n^N|a_{\mathbf{p}}|E_m^{N+1}\rangle\langle E_m^{N+1}|a_{\mathbf{p}}^\dagger|E_n^N\rangle \tag{18}$$

$$=-\frac{1}{Z}\sum_{N,n,m}e^{-\beta(E_n^N-\mu N)}\frac{1\mp e^{-\beta(E_m^{N+1}-E_n^N-\mu)}}{i\omega_k+E_n^N-E_m^{N+1}+\mu}|\langle E_n^N|a_{\mathbf{p}}|E_m^{N+1}\rangle|^2 \tag{19}$$

In particular, we see, that the single-particle excitation energies of the system $E_m^{N+1}-E_n^N-\mu$ are contained in the denominator, which can be made more explicit introducing the spectral function, Γ,

$$A(\mathbf{p},\omega) \;=\; \text{Im}\;\mathcal{G}(\mathbf{p};i\omega_k\to\omega+i\eta) \tag{20}$$

$$\;=\;\frac{1}{Z}\sum_{N,n,m}e^{-\beta(E_n^N-\mu N)}\left(1\mp e^{-\beta\omega}\right)|\langle E_n^N|a_{\mathbf{p}}|E_m^{N+1}\rangle|^2 2\pi\delta(\omega-E_m^{N+1}+E_n^N+\mu) \tag{21}$$

with ω real, and we have

$$\mathcal{G}(\mathbf{p},i\omega_k)=-\int\frac{d\omega'}{2\pi}\frac{A(\mathbf{p},\omega')}{i\omega_k-\omega'} \tag{22}$$

Time dependent Green's function. We can analytically continue the finite-temperature Green's function to "real time", $\tau\to it\pm\eta$. In the limit $\eta\to0$, it is important to consider the corresponding Green's function (upper or lower line of Eq. (17)). The spectral function determines also the real time response of the system.

Self-energy, effective mass. Let us look at the exact one-particle Green's function which can be written as

$$G^{-1}(\mathbf{k},z) = z - \zeta_k - \Sigma(\mathbf{k},z) \tag{23}$$
$$\zeta_k = \varepsilon_k - \mu \tag{24}$$

We have seen before, that the poles of the analytic continuation, in particular the spectral function, enters into the Fermi-function in a similar way as the exact single particle energies for the ideal Fermi gas. Let us continue approach the real axis from above for the self-energy

$$\Sigma(\mathbf{k},\omega) \equiv \Sigma(\mathbf{k}, z = \omega + i\eta) \tag{25}$$

and separate real and imaginary parts

$$G^{-1}(\mathbf{k},\omega) = \omega - [\zeta_k + \mathrm{Re}\,\Sigma(\mathbf{k},\omega)] - i\,\mathrm{Im}\,\Sigma(\mathbf{k},\omega) \tag{26}$$

The poles of the Green's function, and thus the single particle excitation energies, are determined by $G^{-1}(\mathbf{k},\epsilon_k) = 0$. We might expect that $\epsilon_k \approx \zeta_k \approx 0$. Neglecting the imaginary part of the self-energy for a moment, we expect that we can expand the real part of the self-energy around ζ_{k_F}, and k around k_F. We get

$$G(\mathbf{k},\omega) \approx \frac{Z}{\omega - \widetilde{\zeta}_k} \tag{27}$$
$$Z^{-1} = 1 - \left.\frac{\partial \mathrm{Re}\,\Sigma(k_F,\omega)}{\partial\omega}\right|_{\omega=0} \tag{28}$$
$$\widetilde{\zeta}_k = \frac{(k-k_F)k_F}{m^*} \tag{29}$$
$$\frac{1}{m^*} = \frac{Z}{k_F}\left.\frac{\partial[\zeta_k + \mathrm{Re}\,\Sigma(k_F,0)]}{\partial k}\right|_{k=k_F} \tag{30}$$

In contrast to the ideal gas where $\zeta_k \simeq (k-k_F)k_F/m$ close to k_F, the system behaves similar to an ideal gas, but with an effective mass m^*. Further, the weight of the excitation is reduced from one to $Z \leq 1$, but we still have a delta-peak in the spectral function writes

$$A(\mathbf{k},\omega) = 2\pi Z \delta(\omega - \widetilde{\zeta}_k) \tag{31}$$

However the general sum rule

$$\int \frac{d\omega}{2\pi} A(k,\omega) = 1 \tag{32}$$

is not anymore satisfied, due to a incoherent part in the spectral function which is connected to the imaginary part of the self energy.

In general, these expansions are only valid if the imaginary part of the self energy is neglegible. One might expect that this is the case for the electron gas for excitations close to the Fermi-surface, since the Pauli-factors reduce dramatically the avaiable phase space for incoherent scattering. Whenever, the imaginary part is sufficiently small, we can speak of a Fermi liquid, where many properties behave similar to the ideal Fermi gas.

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