3. Exercise on QFT for many-body systems

29/04/2016

5. Fermi liquid parameters from microscopic theories 1+2+1=4 points

In interacting microscopic theories one of the most important quantities is, arguably, the selfenergy $\Sigma(\vec{k},\omega)$. In the lecture it was shown that for a metal one can connect values extracted out of a Taylor expansion of the self-energy around the Fermi level to the phenomenological parameters of the Landau Fermi liquid (FL) theory.

In particular, if the self-energy out of the microscopic theory considered (e.g. dynamical mean field theory) is purely local [i.e., not \vec{k} -dependent: $\Sigma(\vec{k},\omega) = \Sigma(\omega)$], one obtains the following relations:

$$Z = \left[1 - \frac{\partial \operatorname{Re} \Sigma(\omega)}{\partial \omega}\Big|_{\omega \to 0}\right]^{-1}, \quad \frac{m^*}{m} = Z^{-1}, \quad \Gamma = -\operatorname{Im} \Sigma(\omega)\Big|_{\omega \to 0}$$
(1)

where Z is the quasiparticle weight, m^* the effective mass and Γ defines the quasiparticle scattering rate so that the quasiparticle lifetime is $\tau = (2Z\Gamma)^{-1}$.

Now consider the file siwdat.txt. It contains local fermionic self-energies on the positive Matsubara axis $\Sigma_c(i\nu_n)$ for four different physical cases c = 1, 2, 3, 4 at the inverse temperature $\beta = 50 \text{ eV}^{-1}$. The format of the columns in the file is ν_n — Re $\Sigma_1(i\nu_n)$ — Im $\Sigma_1(i\nu_n)$ — Re $\Sigma_2(i\nu_n)$...

- a) Plot the real and imaginary parts of the self-energies in all cases, respectively.
- **b)** For cases one to three numerically extract the quasiparticle weight Z, the effective mass $\frac{m^*}{m}$ and Γ . What is the difference between these cases and how could one interpret those? *Hint:* In principle one would have to analytically continue the self-energy from the Matsubara to the real frequency axis $(i\nu_n \to \omega + i\delta)$. However, show that these parameters can also be approximately obtained directly at Matsubara as following:

$$Z = \left[1 - \frac{\partial Im \ \Sigma(i\nu_n)}{\partial \nu_n} \Big|_{\nu_n \to 0^+} \right]^{-1}, \quad \Gamma = -Im \ \Sigma(i\nu_n) \Big|_{\nu_n \to 0^+}$$

c) What about the fourth case? See also exercise 6.

6. A very simple model with strong correlations

 $1+3+2=6 \ points$

Landau FL theory, as a theory for metals, reproduces many qualitative features of the noninteracting Fermi gases. In FL systems, the screened Coulomb energy is much smaller than the electronic kinetic energy. As a result, the electron-electron interactions can be treated as small perturbations to the motion of the electrons at the Fermi level.

However, in a different limit, *i.e.* when Coulomb energy is much stronger than the electronic kinetic energy, FL theory will not hold anymore. An intuitive, yet simple, example for understanding the complete disappearance of coherent quasiparticles due to the strong electronelectron correlations is the Hubbard model in the "atomic limit", which reads:

$$H_{\rm at} = U n_{\uparrow} n_{\downarrow} - \mu (n_{\uparrow} + n_{\downarrow}) . \tag{2}$$

Let us consider, here, the half filling case, *i.e.* 1 electron per site, obtained for chemical potential $\mu = \frac{U}{2}$, which we absorb in the Hamiltonian of Eq. (2). We observe that only one energy scale appears in this model, *i.e.* the local Coulomb repulsion U.

As the particle numbers n_{\uparrow} and n_{\downarrow} are good quantum numbers of this Hamiltonian, the basis of the problem can be simply taken as the number basis:

$$|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle,$$
(3)

which represents the empty, singly occupied (with up/down spin) and doubly occupied states, respectively.

- a) Show that the states in Eq. (3) are also the eigenstates of H_{at} and find the corresponding eigenenergies. Show the partition function at inverse temperature β is given as $\mathcal{Z} = \text{Tr}e^{-\beta H} = 2(1 + e^{\beta U/2}).$
- **b)** Try to express the creation and annihilation operators $\hat{c}^{\dagger}_{\sigma}$ and \hat{c}_{σ} as 4×4 matrices in the above basis. Show that the imaginary-time Green's function is given by

$$G_{\sigma}(\tau) = -\langle T_{\tau}\hat{c}_{\sigma}(\tau)\hat{c}_{\sigma}^{\dagger}\rangle = -\frac{1}{\mathcal{Z}}\mathrm{Tr}[e^{-\beta H}\hat{c}_{\sigma}(\tau)\hat{c}_{\sigma}^{\dagger}] = -\frac{e^{\frac{U}{2}\tau} + e^{(\beta-\tau)\frac{U}{2}}}{\mathcal{Z}},\qquad(4)$$

where σ stands for the spin orientation \uparrow (or \downarrow)

c) Fourier transform the imaginary-time Green's function $G_{\sigma}(\tau)$ to Matsubara space to get $G_{\sigma}(i\nu_n) = \int_0^{\beta} G_{\sigma}(\tau) e^{i\nu_n \tau} d\tau$ and determine the corresponding spectral function $A_{\sigma}(\omega)$ and the self-energy $\Sigma_{\sigma}(\omega)$. [Hint: to get $A_{\sigma}(\omega)$ at real frequency axis, an analytical continuation $i\nu_n \to \omega + i\delta$ is required]. Does the system have an energy gap, and if so how large is it? Do we have well-defined quasiparticle in this case? [Hints: try to determine the quasiparticle weight Z, effective mass m^* and scattering rate Γ as defined in Eq. (1).]