Exercises on Introduction of many-body physics of fermions and bosons
Master 2 ICFP

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9 janvier 2021

1 Introduction

1.1 Density of states

We calculate in the introductory chapter the density of states $\rho(\varepsilon)$ for a quadratic dispersion relation.
Perform the same analysis with a linear dispersion relation instead of a quadratic one in dimension $d = 2$ and $d = 3$.

2 Green functions

2.1 Some properties

1. Show that the retarded Green function G^R is a function of $t - t'$.

2. Show that
$$G^M_{ab}(i\omega_n) = \int_{-\beta/2}^{\beta/2} d\tau G^M_{ab}(\tau) e^{i\omega_n \tau}.$$

2.2 Single-level

1. Let us consider the single-particel Hamiltonian
$$\hat{H} = \varepsilon \hat{c}^\dagger \hat{c},$$

Compute the following Green functions
$$G^M(\tau),\ G^M(i\omega_n) \text{ et } G^R(\omega),$$

2. Plot $G^M(\tau)$. What are the values of $G^M(0^+)$ and $G^M(\beta^-)$?
3. Compute the density of states associated to this level.

2.3 Density of states

Show using the Lehman representation that the density of states is normalized, namely that $\int d\omega \rho(\omega) = 1$.

3 Feynman Diagrams

3.1 Simple diagrammatic approach

Consider the Hamiltonian

$$\hat{H} = \sum_k \varepsilon_k \hat{c}_k^\dagger \hat{c}_k + \varepsilon_d \hat{d}^\dagger \hat{d} + \frac{t}{\sqrt{V}} \sum_k \left(\hat{c}_k^\dagger \hat{d} + \text{h.c.} \right).$$

Calculate using a diagrammatic approach the Green function

$$G_d(\tau - \tau') = -\langle T_\tau \hat{d}(\tau) \hat{d}^\dagger(\tau') \rangle = -\frac{\langle T_\tau \tilde{d}(\tau) \tilde{d}(\tau') e^{-\int_0^\beta du \tilde{V}(u)} \rangle}{\langle T_\tau e^{-\int_0^\beta du \tilde{V}(u)} \rangle}.$$

3.2 Fermions in interaction : the bubble diagram

We consider a homogeneous gas of spin 1/2 fermions interacting through a short-range two-body potential $V(\vec{r} - \vec{r}') = g\delta(\vec{r}' - \vec{r})$ with the coupling strength g [1].

The Hamiltonian describing the system reads

$$\hat{H} = \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_k \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} + \frac{g}{\mathcal{V}} \sum_{q,k_1,k_2} \hat{c}_{k_1+q,\uparrow}^\dagger \hat{c}_{k_2-q,\downarrow}^\dagger \hat{c}_{k_2,\downarrow} \hat{c}_{k_1,\uparrow}, \tag{1}$$

where $\mathcal{V}$ is the volume of the system and $\varepsilon_k = \hbar^2 k^2/2m$ is the single-particle spectrum for free fermions. We are interested in the calculation of the fermionic self-energy at second order in g to study the quasi-particles life-time. The first order corresponds to the Hartree and Fock diagrams. The Fock diagram gives a zero contribution because of Pauli's principle combined with a point interaction. The Hartree term gives $\Sigma_\sigma^{(1)}(k, i\omega_n) = gn/2$ where $n = k_F^3/(3\pi^2)$ is the total fermion density. Therefore, $n/2$ is the fermion density for a single fermion species.

The purpose of this exercise is to calculate the contribution of the bubble diagram to the self-energy by focusing on its imaginary part.

1. Show that the corresponding contribution writes as

$$\Sigma_\sigma^{(2)}(k, i\omega_n) = -\frac{g^2}{\beta^2 \mathcal{V}^2} \sum_{k_1,k_2} \sum_{\omega_1,\omega_2} \frac{1}{i\omega_1 - \xi_{k_1}} \frac{1}{i\omega_2 - \xi_{k_2}} \frac{1}{i\omega_3 - \xi_{k_3}}, \tag{2}$$

with conservation rules $\omega_3 = \omega_n + \omega_2 - \omega_1$ et $k_3 = k + k_2 - k_1$. We have introduced the notation $\xi_k = \varepsilon_k - \mu$.

2. Perform the summation over frequencies ω_2 and then over ω_1 (or *vice-versa*), to obtain

$$\Sigma_\sigma^{(2)}(k, i\omega_n) = -\frac{g^2}{\mathcal{V}^2} \sum_{k_1,k_2} \frac{(n_F(\xi_2) - n_F(\xi_3))(n_F(\xi_1) + n_B(\xi_2 - \xi_3))}{i\omega_n + \xi_2 - \xi_1 - \xi_3}, \tag{3}$$

where $n_F(\varepsilon)$ and $n_B(\varepsilon)$are the Fermi and Bose distributions respectively.

3. Now take the analytic continuation $i\omega_n \to \omega + i0^+$ and the imaginary part of the self-energy. After a bit of algebra on the distribution functions, show that

$$\Im\Sigma_\sigma^{(2)}(k, \omega) = -\pi \frac{g^2}{\mathcal{V}^2} \sum_{k_1,k_2} \bar{n}_F(\xi_1) n_F(\xi_2) \bar{n}_F(\xi_3) \delta(\omega + \xi_2 - \xi_1 - \xi_3) \left(1 + e^{-\beta\omega}\right). \tag{4}$$

where $\bar{n}_F(\varepsilon) = 1 - n_F(\varepsilon)$

4. Is it possible to recover this result using the Fermi golden rule ?

5. Instead of computing directly $\Im\Sigma^{(2)}$, we prefer to calculate its mean value by summing over the $\vec{k}$ wave-vector. We assume that this averaging procedure does not modify the ω dependency of the self-energy. At zero temperature, show that

$$\langle \Im\Sigma_\sigma^{(2)}(\omega) \rangle = -\pi g^2 N_0^3 \frac{\omega^2}{2}, \tag{5}$$

where N_0 denotes the density of states at the Fermi energy.

1. The coupling strength can be written in terms of the 2-body scattering length $g = 4\pi\hbar^2 a/m$.

3.3 Landau damping

In this problem, we are interested in the effect of the coupling to an electronic band of a bosonic excitation (for example a spin wave), described by a bosonic field *scalar* ϕ whose Fourier decomposition reads

$$\hat{\phi}(x) = \sum_q \hat{a}_q e^{iqx} + \hat{a}_q^\dagger e^{-iqx},\ \phi(q) = \hat{a}_{-q} + \hat{a}_q^\dagger \tag{6}$$

with $\hat{a}_q^\dagger$ and $\hat{a}_q$ are the canonical *bosonic* creation/annihilation operators verifying $[\hat{a}_q, \hat{a}_{q'}^\dagger] = \delta_{qq'}$. We model the coupling to the metal at *low energy* by the Hamiltonian

$$\hat{H} = \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \sum_k \varepsilon_k \hat{c}_k^\dagger \hat{c}_k + g \sum_{k,q} (\hat{a}_{-q} + \hat{a}_q^\dagger) \hat{c}_k^\dagger \hat{c}_{k+q}$$

where ω_q is the dispersion relation dof the bosonic mode (we assume $\omega_{-q} = \omega_q$), $\varepsilon_k = k^2/2m$ is the dispersion of the electrons $\hat{c}_k^\dagger$, $\hat{c}_k$. In the whole problem, we place ourselves in dimension $d = 3$.

We define the Green function of the field ϕ in imaginary time by

$$D(q,\tau) = -\langle T\hat{\phi}(q,\tau)\hat{\phi}^\dagger(q,0)\rangle$$

where T denotes the time-ordering in imaginary time and $\phi(q,\tau)$ is written in the Heisenberg represenation.

1. Show that D is a β-periodic function of τ.

2. Find an explicit expression of the Green function $D_0(i\ nu_n)$ in the free case ($g = 0$) where the ν_n are the Matsubara frequencies that we will specify.

3. Give the Feynman's rules for the expansion in g, and draw the diagrams for D and G (fermionic Green functions) to second order in g.

4. By analogy with the fermionic case seen in the lecture, show that we can define a self-energy $\Pi(q,\omega)$ for D (also called polarization). Write the corresponding Dyson equation.

5. With a diagrammatic calculation at the lowest order, show that :

$$\Pi(q, i\nu_n) = a \int \frac{d^3k}{(2\pi)^3} \frac{n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})}{i\nu_n + \varepsilon_k - \varepsilon_{k+q}}$$

where a is a coeficient to be determined

6. Find the zero-temperature expansion of the imaginary part of the retarded polarization $\Im\pi_R(q,\nu)$ for $q,\nu \to 0$ in the near-equilibrium regime $|\nu| \ll v_F q$ (where v_F is the Fermi velicity). We remind that : $\pi_R(q,\nu) = \pi(q, i\nu_n \to \nu + i0^+)$.

In the case of a ferromagnetic spin wave, we have $\omega_q = cq^2$ where c is a constant. Using the expression of D, show that the electron coupling induces a damping of these spin waves. Why does this damping vanish at low frequency ?

4 Introduction to quantum impurity models

4.1 Logarithmic divergences in the Kondo problem

We consider the Kondo Hamiltonian defined by :

$$H_K = J\hat{c}^\dagger(x=0)\vec{S}\cdot\hat{\sigma}\hat{c}(x=0), \tag{7}$$

which describes a local magnetic interaction between an impurity $\vec{S}$ and the conduction electron. In what follows, we consider a $S = 1/2$ spin impurity.

Since there is no Wick theormen for spin operators, an alternative strategy is to use an appropriate representation for the spin operators. It is quite natural to write a spin 1/2 in terms of fermionic operators $\vec{S} = d^\dagger_\alpha \vec{\sigma}_{\alpha\beta} d_\beta$ with the constraint $\sum_\alpha d^\dagger_\alpha d_\alpha = 1$. This representation is due to Abrikosov. Although implementing a constraint is doable (using Lagrange multiplier for example), this is not always very convenient.

Another representation which is appropriate here is the Majorana fermion representation. Consider a fermionic operator c and write it $c = (\gamma^a + i\gamma^b)/\sqrt{2}$ and $c^\dagger = (\gamma^a - i\gamma^b)/\sqrt{2}$. Equivalently $\gamma^a = (c + c^\dagger)/\sqrt{2}$ and $\gamma^b = (c - c^\dagger)/i\sqrt{2}$. The operators $\gamma^{a,b}$ are fermionic operators and are self-adjoint : $\gamma^{a,b} = (\gamma^{a,b})^\dagger$. They are called Majorana operators.

1. Show that $\{\eta^a, \eta^b\} = \delta_{ab}$ where η^a, η^b are Majorana operators. Infer that $(\eta^a)^2 = 1/2$.

2. We introduce three Majorana operators η^x, η^y, η^z. We define a spin operator as $S^a = -\frac{i}{2}\epsilon^{abc}\eta^b\eta^c$ where ϵ^{abc} is the totally antisymmetric tensor. Einstein convention is used here. Show that such operator satisfied some SU(2) algebra that is

$$[S^a, S^b] = i\epsilon^{abc}S^c$$

and $\sum_a (S^a)^2 = 3/4$. This implies $S^x = -i\eta^y\eta^z$, $S^y = -i\eta^z\eta^x$ and $S^z = -i\eta^x\eta^y$. Contrary to Abrikosov fermions, there is no constraint to implement here !

3. Because a Majorana fermion squares to a constant, a non-interacting (quadratic) Hamiltonian of Majorana fermions is thus trivial and we can assume $H_{\text{Maj}} = 0$. Therefore the Matsubara Green function for Majorana fermions reduces simply to

$$G_\eta(\tau) = -\langle T_\tau \eta(\tau)\eta(0)\rangle = -1/2$$

Show that $G_\eta(i\omega_n) = 1/(i\omega_n)$.

4. Our Kondo Hamiltonian thus reads :

$$H_K = -\frac{i}{2}J\epsilon^{abc}\eta^b\eta^c\sigma^a_{uv}\hat{c}^\dagger_u(x=0)\hat{c}_v(x=0),$$

where again Einstein convention is assumed here to alledge notations.

The Green function of a Majorana fermion is just a non-oriented straight line because creation and annihilation are similar. The Kondo Hamiltonian is thus an interaction involving four bodies : two normal fermions and two Majorana fermions. This is almost like a problem we dealt with in chapter III. The vertex can thus be represented as in Fig. 1. The Feynmann rules are thus almost similar. In what follows, we assume particle-hole symmetry. This means $\rho(\omega) = \rho(-\omega)$ where ρ denotes the density of states of the conduction electrons. We want to compute how the vertex is modifed in perturbation theory. The bare vertex is already linear in J. Therefore, at second order in J, which means first order in perturbation theory, we can draw two non-trivial diagrams as depicted in Fig. 2.

Write the contribution of the two diagrams in terms of $G_c(\tau)$ and $G_\eta(\tau)$ the Matsubara Green function for the conduction electrons and Majorana fermions respectively.

5. Show that when we add the two diagrams, they combine nicely to give the initial Kondo Hamiltonian provided we define an effective Kondo coupling $J_{eff} = J + 2J^2 \int_0^\beta d\tau [G_c(\tau)G_\eta(\tau)]$.

6. Evaluate the above integral if we choose $\rho(\epsilon) = \rho_0$ for $|\epsilon| \le D$ and $\rho(\epsilon) = 0$ $|\epsilon| > D$. You only need to evaluate the leading divergence. Conclusion ?

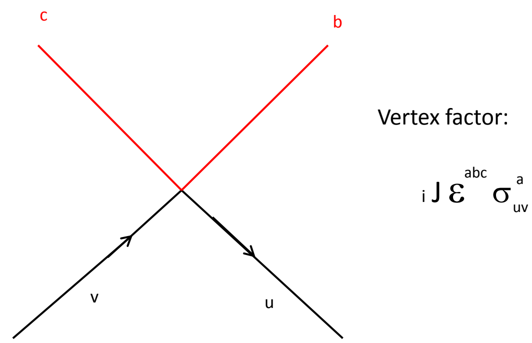

FIGURE 1 – Representation of the vertex. The extra factor 2 comes from the invariance under exchange of b and c in H_K.

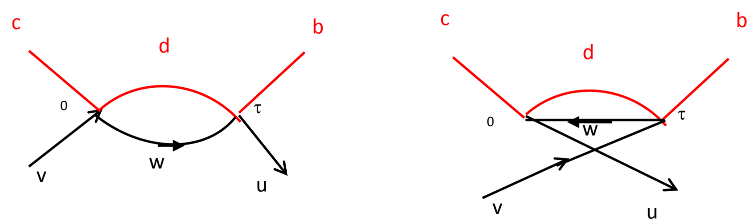

FIGURE 2 – The two diagrams at order J^2. Notice that they are different because of the w propagator which goes from 0 to τ in the 1st one and from τ to 0 in the 2nd one.

4.2 Impurity susceptibility

We are interested in an isolated magnetic impurity immersed in a metal, modeled by the Kondo Hamiltonian

$$\hat{H}_J = \sum_{\alpha=\uparrow,\downarrow} \sum_{\vec{k}} \varepsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k},\alpha} \hat{c}_{\vec{k},\alpha} + J\hat{\vec{S}} \cdot \sum_{\alpha,\alpha'=\uparrow,\downarrow} \hat{c}^\dagger_\alpha(0) \vec{\sigma}_{\alpha\alpha'} \hat{c}_{\alpha'}(0) - h\hat{M}^z, \tag{8}$$

where

$$\hat{M}^z = \hat{S}^z + \sum_{\alpha,\alpha'=\uparrow,\downarrow} \int dx \hat{c}^\dagger_\alpha(x) \frac{\sigma^z_{\alpha\alpha'}}{2} \hat{c}_{\alpha'}(x). \tag{9}$$

The impurity is represented by a spin $\hat{\vec{S}}$, a spin 1/2 localized in $x = 0$, which interacts with a conduction band (the c electrons) via some local antiferromagnetic coupling $J > 0$. We assume the system is in a magnetic field h along the z direction. $\hat{c}^\dagger_\alpha(0) \equiv \hat{c}^\dagger_\alpha(x = 0)$ denotes the creation operator for a conductaion electron in $x = 0$ and $\vec{\sigma}$ are the Pauli matrices.

We are interested in the susceptibility of the impurity defined by

$$\chi_{imp} \equiv \left. \frac{d \langle \hat{M}^z \rangle}{dh} \right|_{h=0} - \chi_{0,Pauli} \tag{10}$$

where $\chi_{0,Pauli}$ is the Pauli susceptibility of the conduction electrons c for $J = 0$. The purpose of this problem is to show that the pertrubative expansion in powers of J of the "Curie constant" $T\chi_{imp}(T)$ has a logarithmic divergence in the $T \to 0$ limit, or more explicitly (a is a constant that will not be determined) that

$$\chi_{imp} = \frac{1}{4T}\left(1 - 2J\rho_0 + (2J\rho_0)^2 \ln\frac{T}{D} + a(J\rho_0)^2\right) + \mathcal{O}(J^3) \tag{11}$$

1. Show the result of (11) to 0^{th} order in J (i.e. a isolated spin). Why is this result correct at high temperature whatever J?

2. For a general Hamiltonian $\hat{H} = \hat{H}_0 + g\hat{H}_{int}$,with a coupling g show that the free energy satisfies :

$$\frac{\partial F}{\partial g} = \langle \hat{H}_{int} \rangle_g \,, \tag{12}$$

where the notation $\langle \cdots \rangle_g$ means the thermodynamical average with respect to the full Hamiltonian with interaction g. Infer that

$$\chi_{imp} = \frac{1}{4T} - \int_0^J d\tilde{J} \frac{\partial^2}{\partial h^2} \left. \langle \hat{\vec{S}} \cdot \hat{c}^\dagger(0)\vec{\sigma}\hat{c}(0) \rangle_{\tilde{J}} \right|_{h=0}. \tag{13}$$

3. We therefore need to calculate the average $\langle \hat{A} \rangle_J$ of $\hat{A} \equiv \hat{\vec{S}} \cdot \hat{c}^\dagger(0)\vec{\sigma}\hat{c}(0)$ with respect to the Kondo Hamiltonian. We will do that in perturbation theory.

Compute χ_{imp} to order 1.

4. Show that $\hat{A} = \hat{S}^z \hat{c}^\dagger(0)\sigma^z\hat{c}(0) + (\hat{S}^+ \hat{c}_\downarrow^\dagger(0)\hat{c}_\uparrow(0) + \hat{S}^- \hat{c}_\uparrow^\dagger(0)\hat{c}_\downarrow(0))$

5. Calculate explicitly the correlation function $\langle T_\tau \hat{S}^a(\tau)\hat{S}^b(0) \rangle_0$ where $a, b = z, +, -$ in presence of a magnetic field h.

6. Compute the correlators involving $\hat{c}$, $\hat{c}^\dagger$ using the Wick theorem.

7. Can you infer χ_{imp} to second order 2 if you *keep only the divergent term*?