Problem set 5 - Many-body theory SFI7534

For correction, return only those problems marked with $\star$.

1. **Grand partition function of quantum gases**
   In class, we have computed the grand partition function for ideal quantum gases using the formalism of path integrals in the continuum limit. In that case, a frequency sum over Matsubara frequencies had to be carefully performed. The purpose of this problem is to rederive this result without taking the continuum limit.

   (a) Firstly, rederive the field integral for the many-body grand partition function without taking the continuum limit. For this, consider $H_0 = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha$, and show that the corresponding grand-partition is

   $$Q_0 = \lim_{M\to\infty} \prod_\alpha \left(\int \prod_k \frac{1}{N} \mathrm{d}\bar{\psi}_k \mathrm{d}\psi_k e^{-\bar{\boldsymbol{\psi}}^T \cdot \mathbb{S}^{(\alpha)} \cdot \boldsymbol{\psi}} \right),$$

   with the matrix

   $$\mathbb{S}^{(\alpha)} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & -\zeta c_\alpha \\ -c_\alpha & 1 & 0 & \cdots & 0 & 0 \\ 0 & -c_\alpha & 1 & \cdots & 0 & 0 \\ 0 & 0 & -c_\alpha & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 & 0 \\ 0 & 0 & 0 & \cdots & -c_\alpha & 1 \end{pmatrix}, \text{ and } c_\alpha = 1 - \frac{\beta}{M}(\epsilon_\alpha - \mu).$$

   Define carefully what is $\bar{\psi}_k$, ψ_k, M, β, ζ, and N. Moreover, what are the possible values of k in the productory? Is there a need of adding an index α in $\bar{\psi}_k$ and ψ_k? Why? How about the interacting case?

   (b) Perform the Gaussian integral and take the limit $M \to \infty$ to arrive at the desired result. (Notice there was no need in performing a Matsubara frequency sum.)

2. **Non-interacting Green's function**
   Let us now compute the single-particle Green's function for noninteracting systems in the same philosophy as in the previous problem. Here

   $$\mathcal{G}_0(\alpha, \tau_q; \gamma, \tau_r) = \frac{1}{Q_0} \mathrm{tr}\left\{ T e^{-\int_0^\beta \mathrm{d}\tau (H_0 - \mu N)} a_\alpha(\tau_q) a_\gamma^\dagger(\tau_r) \right\},$$

   with $\tau_x = x\frac{\beta}{M}$ corresponding to the time in the x-th time slice (with $x = q, r$ integer).

   (a) Show that

   $$\mathcal{G}_0(\alpha, \tau_q; \gamma, \tau_r) = \left(\left(\mathbb{S}^{(\alpha)} \right)^{-1} \right)_{q,r} \delta_{\alpha,\gamma},$$

   where

   $$\left(\mathbb{S}^{(\alpha)} \right)^{-1} = \frac{1}{1 - \zeta c_\alpha^M} \begin{pmatrix} 1 & \zeta c_\alpha^{M-1} & \zeta c_\alpha^{M-2} & \cdots & \zeta c_\alpha^2 & \zeta c_\alpha \\ c_\alpha & 1 & \zeta c_\alpha^{M-1} & \cdots & \zeta c_\alpha^3 & \zeta c_\alpha^2 \\ c_\alpha^2 & c_\alpha & 1 & \cdots & \zeta c_\alpha^4 & \zeta c_\alpha^3 \\ c_\alpha^3 & c_\alpha^2 & c_\alpha & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 & \zeta c_\alpha^{M-1} \\ c_\alpha^{M-1} & c_\alpha^{M-2} & c_\alpha^{M-3} & \cdots & c_\alpha & 1 \end{pmatrix}.$$

   (b) In the limit $M \to \infty$, show that

   $$\left(\left(\mathbb{S}^{(\alpha)} \right)^{-1} \right)_{q,r} \to \begin{cases} e^{-(\epsilon_\alpha - \mu)(\tau_q - \tau_r)} (1 + \zeta n_\alpha), & \text{for } q \geq r, \\ e^{-(\epsilon_\alpha - \mu)(\tau_q - \tau_r)} \zeta n_\alpha, & \text{otherwise,} \end{cases} \quad \text{with, } n_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - \zeta}$$

   being the mean occupation number. Therefore, the Green's function can be compactly written as $\mathcal{G}_0(\alpha, \tau; \alpha', \tau') = \delta_{\alpha,\alpha'} g_\alpha(\tau - \tau' + \eta)$, with $\eta \to 0^+$. What is the expression for g_α?

3. $\star$ **Feynman diagrams for external local potential at $T \neq 0$ (see Fetter+Walecka probs. 7.4 and 7.5)** Consider a system of noninteracting particles in a local external static potential given by $H^{\text{ext}} = \int \mathrm{d}\mathbf{x} \psi_\alpha^\dagger(\mathbf{x}) V_{\alpha,\beta}(\mathbf{x}) \psi_\beta(\mathbf{x})$.

   (a) Use Wick's theorem to evaluate the Matsubara Green's function to second order in H^{ext}, and thus, deduce the Feynman rules for $\mathcal{G}^{\text{ext}}_{\alpha,\beta}(x,y)$ to all orders (where $x = \mathbf{x}, \tau_x$).

   (b) Define the Fourier transform

   $$\mathcal{G}^{\text{ext}}_{\alpha,\beta}(x,y) = \frac{1}{\beta\hbar}\sum_n \int\int \frac{\mathrm{d}\mathbf{k}\mathrm{d}\mathbf{q}}{(2\pi)^6} e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{y}-\omega_n(\tau_x-\tau_y))}\mathcal{G}^{\text{ext}}_{\alpha,\beta}(\mathbf{k},\mathbf{q},\omega_n).$$

   Find $\mathcal{G}^{\text{ext}}_{\alpha,\beta}(\mathbf{k},\mathbf{q},\omega_n)$ to second order, and hence obtain the corresponding Feynman rules in momentum space.

   (c) Show that Dyson's equation becomes

   $$\mathcal{G}^{\text{ext}}_{\alpha,\beta}(\mathbf{k},\mathbf{q},\omega_n) = \mathcal{G}^{(0)}_{\alpha,\beta}(\mathbf{k},\omega_n)(2\pi)^3\delta(\mathbf{k}-\mathbf{q}) + \int \frac{\mathrm{d}\mathbf{p}}{(2\pi)^3\hbar}\mathcal{G}^{(0)}_{\alpha,\lambda}(\mathbf{k},\omega_n)V_{\lambda,\delta}(\mathbf{k}-\mathbf{p})\mathcal{G}^{\text{ext}}_{\delta,\beta}(\mathbf{p},\mathbf{q},\omega_n).$$

   (d) Compute the internal energy $\langle E\rangle$ and the grand thermodynamical potential Ω in terms of the Green's function.
   Now, lets consider a system of spin-1/2 fermions in a uniform magnetic field: $V_{\alpha,\beta}(\mathbf{x}) = -\mu_0\mathbf{B}\cdot\boldsymbol{\sigma}_{\alpha,\beta}$.

   (e) Express the magnetization $\mathbf{M} = \frac{1}{2}\mu_0\langle\boldsymbol{\sigma}\rangle$ in terms of the zero-temperature G^{ext} and finite-temperature $\mathcal{G}^{\text{ext}}$ Green's function.

   (f) Solve Dyson's equation in each case and find $\mathbf{M}$. Compute the susceptibility and discuss the limits $T \to 0$ (Pauli paramagnetism) and $T \to \infty$ (Curie's law).

4. **Path integral for an Harmonic Oscillator**
   Consider the 1D quantum Harmonic Oscillator given by the Hamiltonian

   $$H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 Q^2.$$

   (a) Derive the corresponding path integral and show that, in the continuum limit,

   $$Z = \mathrm{tr}e^{-\beta H} = \int \mathcal{D}[q(\tau)]e^{-S_E[q]}, \text{ with } S_E = \int_0^\beta \mathrm{d}\tau\left(\frac{m}{2}\dot{q}^2 + \frac{1}{2}m\omega^2 q^2\right).$$

   What is the exact expression for $\mathcal{D}[q(\tau)]$?

   (b) Now, let us step back and work on the driscret case. Defining the Fourier transform

   $$\tilde{q}_k = \frac{1}{\sqrt{M}}\sum_j e^{-2\pi ijk/M}q_j, \text{ and } q_j = \frac{1}{\sqrt{M}}\sum_k e^{2\pi ijk/M}q_j,$$

   show that

   $$S_E = \epsilon\sum_k \tilde{q}_k\left[\frac{1}{2}m\omega^2 + \frac{m}{\epsilon^2}\left(1-e^{-2\pi ik/M}\right)\right]\tilde{q}_{-k}, \text{ with } \epsilon = \beta/M.$$

   (c) Finally, show that

   $$Z = \frac{1}{2\sinh\left(\frac{1}{2}\beta\omega\right)}.$$

   (d) Performing an analytical continuation of the Euclidean time to the Minkowski time $\beta \to it$, show that

   $$Z_M(t) = \frac{1}{2i\sin(\frac{1}{2}\omega t)} = \sum_n e^{-itE_n}, \text{ with } E_n = \left(n+\frac{1}{2}\right)\omega,$$

   which is the Harmonic Oscillator spectrum. Why is that so?

5. ⋆ **Intermediate coupling**
Consider the following Euclidean action

$$S = A\left[\bar{\psi},\psi\right] + B\left[\phi\right] + C\left[\bar{\psi},\psi,\phi\right],$$

where

$$A\left[\bar{\psi},\psi\right] = \int \mathrm{d}\mathbf{k}\mathrm{d}\omega\bar{\psi}_{\mathbf{k},\omega}\left(\xi_{\mathbf{k}} - i\omega\right)\psi_{-\mathbf{k},-\omega},\ B\left[\phi\right] = \int \mathrm{d}\mathbf{k}\mathrm{d}\omega\phi_{\mathbf{k},\omega}\left(m + |\mathbf{k}|^s\right)\phi_{-\mathbf{k},-\omega},$$

$$\text{and } C\left[\bar{\psi},\psi,\phi\right] = g\int \mathrm{d}\mathbf{k}\mathrm{d}\omega\phi_{\mathbf{k},\omega}\rho_{-\mathbf{k},-\omega},\ \text{with } \rho_{\mathbf{k},\omega} = \sum_{\mathbf{q},\nu}\bar{\psi}_{\mathbf{q},\nu}\psi_{\mathbf{p}+\mathbf{q},\omega+\nu}.$$

Here, ϕ is a scalar field, and m, s (usually equal to 1 or 2), and g are constants. Consider 3 spatial dimensions.

(a) Provide an interpretation for each term in S.
(b) For $g = 0$, compute the correlation function $\langle\phi(0,0)\phi(r,\tau)\rangle$ for large r. What is the role of m?
(c) Yet for $g = 0$, what is the the correlation function for $m = 0$ and large r?
(d) For $g \neq 0$, integrate over ϕ and give a physical interpretation of the effective action. (Discuss the cases $m = 0$ and $\neq 0$.)

6. ⋆ **When mean field becomes exact**
In class, we studied the Bose-Hubbard model with nearest-neighbor hopping. Here, let us consider the same model with infinite range hopping

$$H = -\frac{J}{N}\sum_{i,j} b_i^\dagger b_j - \mu\sum_i b_i^\dagger b_j + \frac{1}{2}U\sum_i b_i^\dagger b_i^\dagger b_i b_i,$$

with J and $U > 0$ being constantes. Here, the hopping sum is irrestricted for all possible i,j pairs of a d-dimensional hypercubic lattice of $N \gg 1$ sites.

(a) Why is the hopping term divided by N? (*Hint*: Energy is an extensive quantity.)
(b) In this problem, we want (for a change) work in the real time t formalism instead of the imaginary time τ one. What is the corresponding Minkowski action $S_{\mathrm{M}}\left[\psi,\bar{\psi}\right]$ of this model?
(c) In the corresponding path integral $Z\int\mathcal{D}\left[\psi,\bar{\psi}\right]e^{iS_{\mathrm{M}}}$, introduce an auxiliar Hubbard-Stratonovich complex field $\Delta(t)$ such that decouples the hopping between different sites and that $\langle\psi_j\rangle = \frac{1}{N}\left\langle\sum_j\psi_j\right\rangle = \frac{1}{J}\langle\Delta\rangle$.
(d) Integrate out the bosons and show that the resulting effective action for the Δ field is

$$\int\mathcal{D}\left[\Delta,\bar{\Delta}\right]e^{iS_{\mathrm{eff}}} = \int\mathcal{D}\left[\Delta,\bar{\Delta}\right]e^{iNs_{\mathrm{eff}}} = \int\mathcal{D}\left[\Delta,\bar{\Delta}\right]e^{iN\left(W - \frac{1}{J}\int\mathrm{d}t\bar{\Delta}\Delta\right)},$$

where $W = -i\ln\left(\int\mathcal{D}\left[\psi,\bar{\psi}\right]e^{i\int\mathrm{d}t\left[\bar{\psi}(i\partial_t+\mu)\psi - \frac{1}{2}U\bar{\psi}\bar{\psi}\psi\psi + \Delta\bar{\psi} + i\bar{\Delta}\psi\right]}\right)$.

(e) In class, we were interested in minimizing the effective Euclidean action. Here, we will be interested in maximizing S_{eff}. Are these procedures in odds with each othere? Explain.
(f) Expanding s_{eff} in second order for Δ yields exact results in the limit $N \to \infty$. Explain why this is true. (*Hint*: recall the method of steepest descent.) In this case, mean field becomes exact. Why is this expected?
(g) Expand W up to second order in Δ, show that $W \approx -\int\mathrm{d}t\mathrm{d}t'\bar{\Delta}(t')\Delta(t)\Gamma(t,t')$, $\Gamma(t,t') = -i\left\langle T\psi(t')\bar{\psi}(t)\right\rangle$ is a time-ordered zero-temperature single's particle Green's function. What is the associated Hamiltonian. Show that in the Fourier space

$$\tilde{\Gamma}(\mathbf{k},\omega) = \left(\frac{n+1}{\omega-\epsilon^+} - \frac{n}{\omega+\epsilon^-}\right),$$

where n (to be found) is the number of bosons in the ground state of the associated Hamiltonian and $\epsilon^\pm$ (to be found) are the energy cost for adding and removing a particle, respectively.

(h) Compute the phase diagram in the μ/U *vs.* J/U plane.

(i) Compute the excitation energy spectrum in the Mott insulator phase as well as in the superfluid phase. Why the spectrum is momentum independent? Comment on the Goldstone mode.

7. **The Cooper instability**
Consider two attractively interacting fermions with opposite spin. Imagine that they move in the presence of a gas of fermions filling a Fermi sphere. However, neglect the interactions between them and the fermions filling the Fermi sphere. Thus the role of the fermions filling the sphere is simply to restrict the momenta of the interacting fermions to lie above the Fermi momentum. Such fermions, as Leon Cooper showed, [1] can form a bound state even when the interactions are arbitrarily weak. In this problem, we will consider a simplified delta-interaction to explore this phenomenum. (This was very important for the development of the BCS theory once we realize that these Cooper pairs, which are boson, can condense.)

(a) Consider first the problem of two electrons interacting in vacuum. The Hamiltonian is simply

$$H = \frac{p_1^2 + p_2^2}{2m} - \lambda\delta\left(\mathbf{r}_1 - \mathbf{r}_2\right),$$

with $\lambda > 0$ (attractive). To solve this problem, it is convenient to work on the center of mass reference frame. Then, Fourier transform the corresponding Schrödinger equation and find the equation that determines the bound state energy. (It will depend on a momentum cutoff; define it as Λ.) Finally, show that a bound-state solution is possible only if $\lambda > \lambda_c$, where λ_c (to be found) depends on m and Λ.

(b) Now, let us consider the problem of two electrons in a Fermi sea. As we have argued, the role of the Fermi sphere is to restrict the momenta of these two electrons. Furthermore, as the attractive interaction is mediated by phonons, the natural cutoff Λ is the Debye wavevector which is related to the Debye frequency ω_D. Redo your calculations of item (a) and show that there is a bound state for any $\lambda > 0$. Notice the differences with respect to the previous item. The electrons now scatter out and into states that have energies between E_F and $E_F + \hbar\omega_D$. Finally, show that the binding energy is $|E| \approx 2\hbar\omega_D e^{-\frac{2}{\lambda\rho_F}}$, where ρ_F is the single-particle density of state per volume at the Fermi level. (Use that $E_F \gg \hbar\omega_D$ and that $\lambda \ll 1$.)

(c) Explain using simple arguments how is it possible to always lower the energy by binding the electrons into Cooper pairs when a well defined Fermi surface is present? (Do not forget to use the fact that the interaction is short-ranged.)

(d) What is the maximum current density that such Cooper pairs can carry? (Recall $\mathbf{J} = nq\mathbf{v}$, where n is the density of charge carriers of charge q with velocity $\mathbf{v}$.)

(e) Importantly, we would like to analyze the wavefucntion symmetry of this bound state. The orbital part is symmetric or antisymmetric: $\psi\left(\mathbf{r}_1, \mathbf{r}_2\right) = \pm\psi\left(\mathbf{r}_2, \mathbf{r}_1\right)$? What is the consequence for the spin configuration of this Cooper pair?

(f) Show the mean-square radius of a Cooper pair is

$$\xi^2 = \frac{\int \mathrm{d}\mathbf{r} r^2 \left|\psi\left(\mathbf{r}\right)\right|^2}{\int \mathrm{d}\mathbf{r} \left|\psi\left(\mathbf{r}\right)\right|^2} = \frac{4}{3}\left(\frac{\hbar v_F}{|E|}\right)^2,$$

where $|E|$ is the Cooper pair binding energy and v_F is the Fermi velocity.

[1] L. N. Cooper, Phys. Rev. **104**, 1189 (1956).