RG Methods in Statistical Field Theory: Problem Set 11 Solution

In this problem we will examine the phenomenon of *Pauli paramagnetism* arising from the interaction between a magnetic field and the spins of electrons hopping on a lattice. The derivation allows us to practice the contour integral technique for evaluating Matsubara frequency sums.

Consider a Hamiltonian describing electrons hopping on a d-dimensional lattice:

$$\mathcal{H}_0 = \sum_{ij} \sum_{\sigma} c^\dagger_{i\sigma}(K_{ij} - \mu\delta_{ij})c_{j\sigma}$$

The main difference from the noninteracting spinless fermion case discussed in class is that here our creation/destruction operators have an extra index $\sigma = \uparrow, \downarrow$ describing the spin of the electron. The matrix components K_{ij} have the property that they depend only on the distance between lattice sites: $K_{ij} = K(|\mathbf{x}_i - \mathbf{x}_j|)$. To describe the interaction between the electron spins and a magnetic field B along the $+z$ direction, we add the following term:

$$\mathcal{H}_I = -\frac{1}{2}\mu_0 B \sum_i (n_{i\uparrow} - n_{i\downarrow})$$

where $\mu_0 = e\hbar/2mc$ is the Bohr magneton and $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$ is the number operator counting the electrons with spin σ at site i. This interaction term is easy to interpret: if at a site i we have an $\uparrow$ electron aligned with the magnetic field, the energy is decreased by $\frac{1}{2}\mu_0 B$. If we have a $\downarrow$ electron aligned opposite to the magnetic field, the energy is increased by the same amount.

(a) To simplify the problem, let us transform to the momentum representation. As in class, we substitute the Fourier expansions of the $c_{i\sigma}$ and $c^\dagger_{i\sigma}$ operators:

$$c_{i\sigma} = \frac{1}{N}\sum_{\mathbf{q}\in\text{B.Z.}} e^{i\mathbf{q}\cdot\mathbf{x}_i} c_{\mathbf{q}\sigma} \qquad c^\dagger_{i\sigma} = \frac{1}{N}\sum_{\mathbf{q}\in\text{B.Z.}} e^{-i\mathbf{q}\cdot\mathbf{x}_i} c^\dagger_{\mathbf{q}\sigma}$$

Here $c^\dagger_{\mathbf{q}\sigma}$ and $c_{\mathbf{q}\sigma}$ are creation/destruction operators for an electron with momentum $\mathbf{q}$ and spin σ. Show that the full Hamiltonian can be written as:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I = \frac{1}{N}\sum_{\mathbf{q},\sigma} c^\dagger_{\mathbf{q}\sigma}(E_\mathbf{q} - \mu - \frac{1}{2}\mu_0 B m_\sigma)c_{\mathbf{q}\sigma}$$

where $m_\sigma = 1$ and -1 for $\sigma = \uparrow$ and $\downarrow$ respectively. The energies $E_\mathbf{q}$ are defined through the eigenvalue equation for the K matrix:

$$\sum_j K_{ij} e^{i\mathbf{q}\cdot\mathbf{x}_j} = E_\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{x}_i}$$

Remember the orthonormality relation $\sum_i e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{x}_i} = N\delta_{\mathbf{q}',\mathbf{q}}$.

Answer: Using the fact that

$$\mathcal{H}_I = -\frac{1}{2}\mu_0 B \sum_i (n_{i\uparrow} - n_{i\downarrow}) = -\frac{1}{2}\mu_0 B \sum_{ij}\sum_{\sigma} m_\sigma \delta_{ij} c^\dagger_{i\sigma} c_{i\sigma}$$

we can write:

$$\begin{aligned}
\mathcal{H} &= \sum_{ij}\sum_{\sigma} c^\dagger_{i\sigma}(K_{ij} - \mu\delta_{ij} - \frac{1}{2}\mu_0 B m_\sigma \delta_{ij}) c_{j\sigma} \\
&= \frac{1}{N^2}\sum_{\mathbf{q},\mathbf{q}'}\sum_{ij}\sum_{\sigma} e^{i\mathbf{q}'\cdot\mathbf{x}_j - i\mathbf{q}\cdot\mathbf{x}_i} c^\dagger_{\mathbf{q}\sigma}(K_{ij} - \mu\delta_{ij} - \frac{1}{2}\mu_0 B m_\sigma \delta_{ij}) c_{\mathbf{q}'\sigma} \\
&= \frac{1}{N^2}\sum_{\mathbf{q},\mathbf{q}'}\sum_{i}\sum_{\sigma} e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{x}_i} c^\dagger_{\mathbf{q}\sigma}(E_{\mathbf{q}} - \mu - \frac{1}{2}\mu_0 B m_\sigma) c_{\mathbf{q}'\sigma} \\
&= \frac{1}{N}\sum_{\mathbf{q}}\sum_{\sigma} c^\dagger_{\mathbf{q}\sigma}(E_{\mathbf{q}} - \mu - \frac{1}{2}\mu_0 B m_\sigma) c_{\mathbf{q}\sigma}
\end{aligned}$$

(b) Let us now write the partition function as a functional path integral. For each operator $c^\dagger_{\mathbf{q}\sigma}$ and $c_{\mathbf{q}\sigma}$ we introduce the Grassmann functions $\bar{\psi}_{\mathbf{q}\sigma}(\tau)$ and $\psi_{\mathbf{q}\sigma}(\tau)$. The partition function Z is given by:

$$Z = \int e^S \prod_{\mathbf{q},\sigma} \mathcal{D}\bar{\psi}_{\mathbf{q}\sigma}\mathcal{D}\psi_{\mathbf{q}\sigma}$$

where the action S is:

$$S = \int_0^\beta d\tau \left(-\frac{1}{N}\sum_{\mathbf{q},\sigma} \bar{\psi}_{\mathbf{q}\sigma}(\tau)\frac{\partial}{\partial\tau}\psi_{\mathbf{q}\sigma}(\tau) - \mathcal{H}[\bar{\psi},\psi] \right)$$

Here $\mathcal{H}[\bar{\psi},\psi]$ is the Hamiltonian $\mathcal{H}$ with $c^\dagger_{\mathbf{q}\sigma}$ replaced by $\bar{\psi}_{\mathbf{q}\sigma}(\tau)$ and $c_{\mathbf{q}\sigma}$ replaced by $\psi_{\mathbf{q}\sigma}(\tau)$. Transform to the Matsubara frequency representation and show that the action S becomes:

$$S = \frac{\beta}{N}\sum_{\mathbf{q},\sigma,n} \bar{\psi}_{\mathbf{q}\sigma n}(i\omega_n - E_{\mathbf{q}} + \mu + \frac{1}{2}\mu_0 B m_\sigma)\psi_{\mathbf{q}\sigma n}$$

Here $\bar{\psi}_{\mathbf{q}\sigma n}$ and $\psi_{\mathbf{q}\sigma n}$ are shorthand notation for $\bar{\psi}_{\mathbf{q}\sigma}(\omega_n)$ and $\psi_{\mathbf{q}\sigma}(\omega_n)$.

Answer: The Matsubara frequency representation is defined through:

$$\bar{\psi}_{\mathbf{q}\sigma}(\tau) = \sum_n e^{i\omega_n\tau}\bar{\psi}_{\mathbf{q}\sigma n} \qquad \psi_{\mathbf{q}\sigma}(\tau) = \sum_n e^{-i\omega_n\tau}\psi_{\mathbf{q}\sigma n}$$

Plugging these into the action S, we find:

$$S = \int_0^\beta d\tau \left(-\frac{1}{N}\sum_{\mathbf{q},\sigma} \bar{\psi}_{\mathbf{q}\sigma}(\tau)\frac{\partial}{\partial\tau}\psi_{\mathbf{q}\sigma}(\tau) - \frac{1}{N}\sum_{\mathbf{q},\sigma} \bar{\psi}_{\mathbf{q}\sigma}(\tau)(E_{\mathbf{q}} - \mu - \frac{1}{2}\mu_0 B m_\sigma)\psi_{\mathbf{q}\sigma}(\tau) \right)$$

$$= \frac{1}{N} \sum_{\mathbf{q},\sigma} \sum_{n,m} \int_0^\beta d\tau\, e^{i(\omega_n - \omega_m)\tau} \bar{\psi}_{\mathbf{q}\sigma n} \left(i\omega_m - E_{\mathbf{q}} + \mu + \frac{1}{2}\mu_0 B m_\sigma \right) \psi_{\mathbf{q}\sigma m}$$

$$= \frac{\beta}{N} \sum_{\mathbf{q},\sigma,n} \bar{\psi}_{\mathbf{q}\sigma n} \left(i\omega_n - E_{\mathbf{q}} + \mu + \frac{1}{2}\mu_0 B m_\sigma \right) \psi_{\mathbf{q}\sigma n}$$

(c) The partition function $Z = \int e^S \prod_{\mathbf{q},\sigma,n} d\bar{\psi}_{\mathbf{q}\sigma n}\, d\psi_{\mathbf{q}\sigma n}$ is now easy to evaluate using Grassmann integration rules. You should find the following result for Z:

$$Z = \prod_{\mathbf{q},n} \frac{\beta^2}{N^2} \left((-i\omega_n + E_{\mathbf{q}} - \mu)^2 - \frac{1}{4}\mu_0^2 B^2 \right)$$

Hint: Remember the Grassmann integral identity $\int \exp(a\bar{\psi}\psi)\, d\bar{\psi}\, d\psi = -a$.

<u>**Answer:**</u>

$$Z = \int e^{\frac{\beta}{N}\sum_{\mathbf{q},\sigma,n} \bar{\psi}_{\mathbf{q}\sigma n}\left(i\omega_n - E_{\mathbf{q}} + \mu + \frac{1}{2}\mu_0 B m_\sigma\right)\psi_{\mathbf{q}\sigma n}} \prod_{\mathbf{q},\sigma,n} d\bar{\psi}_{\mathbf{q}\sigma n}\, d\psi_{\mathbf{q}\sigma n}$$

$$= \prod_{\mathbf{q},\sigma,n} \int e^{\frac{\beta}{N}\bar{\psi}_{\mathbf{q}\sigma n}\left(i\omega_n - E_{\mathbf{q}} + \mu + \frac{1}{2}\mu_0 B m_\sigma\right)\psi_{\mathbf{q}\sigma n}} d\bar{\psi}_{\mathbf{q}\sigma n}\, d\psi_{\mathbf{q}\sigma n}$$

$$= \prod_{\mathbf{q},\sigma,n} \frac{\beta}{N} \left(-i\omega_n + E_{\mathbf{q}} - \mu - \frac{1}{2}\mu_0 B m_\sigma \right)$$

$$= \prod_{\mathbf{q},n} \frac{\beta^2}{N^2} \left(-i\omega_n + E_{\mathbf{q}} - \mu - \frac{1}{2}\mu_0 B \right) \left(-i\omega_n + E_{\mathbf{q}} - \mu + \frac{1}{2}\mu_0 B \right)$$

$$= \prod_{\mathbf{q},n} \frac{\beta^2}{N^2} \left((-i\omega_n + E_{\mathbf{q}} - \mu)^2 - \frac{1}{4}\mu_0^2 B^2 \right)$$

(d) From the free energy $A = -\frac{1}{\beta}\ln Z$ calculate the zero-field magnetic susceptibility $\chi = -\left.\partial^2 A/\partial B^2\right|_{B=0}$. Show that:

$$\chi = -\frac{1}{2}\mu_0^2 k_B T \sum_{\mathbf{q},n} \frac{1}{(-i\omega_n + E_{\mathbf{q}} - \mu)^2}$$

<u>**Answer:**</u>

$$A = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\sum_{\mathbf{q},n} \ln\left[\frac{\beta^2}{N^2} \left((-i\omega_n + E_{\mathbf{q}} - \mu)^2 - \frac{1}{4}\mu_0^2 B^2 \right) \right]$$

$$\frac{\partial A}{\partial B} = -\frac{1}{\beta} \sum_{\mathbf{q},n} \frac{-\frac{1}{2}\mu_0^2 B}{(-i\omega_n + E_{\mathbf{q}} - \mu)^2 - \frac{1}{4}\mu_0^2 B^2}$$

$$\chi = -\left.\frac{\partial^2 A}{\partial B^2}\right|_{B=0} = -\frac{1}{2}\mu_0^2 k_B T \sum_{\mathbf{q},n} \frac{1}{(-i\omega_n + E_{\mathbf{q}} - \mu)^2}$$

(e) Using the complex contour trick discussed in class, evaluate the sum over Matsubara frequencies in the expression for χ. Show that:

$$\chi = -\frac{\mu_0^2}{2} \sum_{\mathbf{q}} f'_F(E_{\mathbf{q}})$$

where $f_F(E) = (e^{\beta(E-\mu)} + 1)^{-1}$ is the Fermi distribution and $f'_F(E) \equiv df_F(E)/dE$.

__**Answer:**__ We want to evaluate the sum $S = \sum_{n=-\infty}^{\infty} h(i\omega_n)$, where $h(z) = (-z + E_{\mathbf{q}} - \mu)^{-2}$. Introducing the counting function $g(z) = \beta/(e^{\beta z}+1)$, we use the complex contour integration trick from class, which states that S is given by:

$$S = \sum_{z_i \in \text{poles of } h(z)} \text{Res}_{z=z_i} \left[h(z)g(z)\right]$$

This result is true if the product $h(z)g(z)$ decays faster than R^{-1} on the big circle $z = Re^{i\theta}$ for $R \to \infty$. Clearly this condition is satisfied, since $h(z) \sim z^{-2}$ for large $|z|$. $h(z)$ has a second-order pole at $z = E_{\mathbf{q}} - \mu$, so:

$$S = \text{Res}_{z=E_{\mathbf{q}}-\mu} \frac{\beta}{(-z + E_{\mathbf{q}} - \mu)^2 (e^{\beta z} + 1)} = -\frac{\beta^2 e^{\beta(E_{\mathbf{q}}-\mu)}}{(e^{\beta(E_{\mathbf{q}}-\mu)} + 1)^2} = \beta f'_F(E_{\mathbf{q}})$$

Thus:

$$\chi = -\frac{1}{2}\mu_0^2 k_B T \sum_{\mathbf{q},n} \frac{1}{(-i\omega_n + E_{\mathbf{q}} - \mu)^2} = -\frac{\mu_0^2}{2} \sum_{\mathbf{q}} f'_f(E_{\mathbf{q}})$$

(f) To understand the physical significance of the result for χ, let us introduce the function $\rho(E) \equiv \sum_{\mathbf{q}} \delta(E - E_{\mathbf{q}})$. This function has the property that $\int_E^{E+\Delta E} \rho(E')dE'$ counts the number of $\mathbf{q}$ modes that have energies $E_{\mathbf{q}}$ between E and $E+\Delta E$. (You can see this simply because the integral over the sum of delta functions $\delta(E - E_{\mathbf{q}})$ will contribute 1 for every $E_{\mathbf{q}}$ that falls in the range between E and $E + \Delta E$.) Thus $\rho(E)$ is called the *single-particle density of states*, and it becomes a continuous function in the thermodynamic limit. It is useful in converting sums over the momentum modes $\mathbf{q}$ to integrals over energy E. Show that χ can be rewritten as:

$$\chi = -\frac{\mu_0^2}{2} \int_{-\infty}^{\infty} dE\, \rho(E) f'_F(E)$$

__**Answer:**__

$$\chi = -\frac{\mu_0^2}{2} \sum_{\mathbf{q}} f'_f(E_{\mathbf{q}}) = -\frac{\mu_0^2}{2} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} dE\, \delta(E - E_{\mathbf{q}}) f'_F(E) = -\frac{\mu_0^2}{2} \int_{-\infty}^{\infty} dE\, \rho(E) f'_F(E)$$

(g) Note that in the limit of small T, the Fermi distribution $f_F(E)$ is essentially equal to 1 for $E < \mu$ and equal to 0 for $E > \mu$. The derivative $f'_E(E)$ is nearly zero everywhere except for a small region around $E = \mu$, in other words for E near $E_F \equiv \mu(T = 0)$. Thus at low temperatures the main contribution to the integral for χ in part (f) will come from modes closest to the Fermi surface. As we argued in class, these are the modes which control the low-energy physics of the system. To see this directly, let us calculate χ at $T = 0$. Show that:

$$\chi(T = 0) = \frac{\mu_0^2}{2}\rho(E_F)$$

Thus $\chi(T = 0)$ is directly proportional to the density of states at the Fermi surface. *Hint:* Use the fact that $d\theta(x)/dx = \delta(x)$, where $\theta(x)$ is the step function: $\theta(x) = 1$ for $x > 0$, and $\theta(x) = 0$ for $x < 0$.

Answer: At $T = 0$ the Fermi distribution becomes a step function: $f_F(E) = \theta(E_F - E)$. Thus $f_F'(E) = -\delta(E_F - E)$. Plugging this into the result of part (f) we find:

$$\chi(T = 0) = \frac{\mu_0^2}{2}\int_{-\infty}^{\infty} dE\, \rho(E)\delta(E_F - E) = \frac{\mu_0^2}{2}\rho(E_F)$$