

Homework #8 — Phys625 — Spring 2002

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Deadline: Thursday, April 18, 2002.

Office: Physics 2314

Turn in homework in the class or put it in
the box on the door of Phys 2314 by 10 a.m.

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Do not forget to write your name and the homework number!

Equation numbers with the period, like (3.25), refer to the equations of the textbook.

Equation numbers without period, like (5), refer to the equations of this homework.

Finite Temperature (Ch. IV)

This homework explores the Matsubara diagram technique for a finite temperature T . From operational point of view, it is the same as the diagram technique at zero temperature with the replacement $\omega \rightarrow i\omega_n$, where ω_n is the Matsubara frequency: $\omega_n = \pi T(2n + 1)$ for fermions and $\omega_n = 2n\pi T$ for bosons (n is an integer).

1. [6 points] *Friedel oscillations in 1D* (See Problem 3 of HW 3)

Consider 1D electron gas occupying semi-infinite space $x > 0$ with impenetrable boundary at $x = 0$. The energy dispersion is $\varepsilon(p) = p^2/2m$, but you may use the linearized electron dispersion law near $\pm p_F$.

Calculate electron density $n(x)$ using Eq. (37.15),

$$n(x) = 2T \sum_n \mathcal{G}(i\omega_n, x, x) e^{i0\omega_n}, \quad (1)$$

where $\mathcal{G}(\omega_n, x_1, x_2)$ is the Matsubara Green function of electrons (see Eq. (37.13)) modified appropriately by the zero boundary conditions at $x = 0$. The factor 2 comes from the spin.

Describe how the Friedel oscillations decay with the distance x at a finite temperature T . Make sure that your answer at $T \rightarrow 0$ reproduces the result of Problem 3 of HW 3.

2. [6 points] *RKKY in 3D* (See Problem 5 of HW 3)

Calculate at a finite temperature T how the effective interaction $f(\mathbf{r}_1 - \mathbf{r}_2)$ between two impurity spins via exchange with the 3D electron gas depends on the distance $|\mathbf{r}_1 - \mathbf{r}_2|$:

$$\hat{H}_{eff} = f(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{S}_1 \cdot \mathbf{S}_2. \quad (2)$$

As in Problem 5 of HW 3,

$$f(\mathbf{r}) \propto T \sum_n \mathcal{G}^2(i\omega_n, \mathbf{r}), \quad (3)$$

where the Matsubara Green function of electrons is given by Eq. (37.13), but you may use the linearized electron dispersion law near p_F .

3. Matsubara density-density correlator [4 points]

Matsubara density-density correlation function for a Fermi gas is defined as

$$\Pi(\mathbf{r} - \mathbf{r}', \tau - \tau') = i \langle \mathcal{T} \hat{n}(\mathbf{r}, \tau) \hat{n}(\mathbf{r}', \tau') \rangle, \quad (4)$$

where \mathcal{T} is the chronological product with respect to the Matsubara time τ .

Derive a general expression for the density-density correlator (4) in the momentum representation, $\Pi(i\Omega_n, \mathbf{q})$. In order to do that, draw the Feynman diagram that corresponds to the calculation of (4) and express $\Pi(i\Omega_n, \mathbf{q})$ in terms of Matsubara Green's functions of the noninteracting electrons, $\mathcal{G}(i\omega_m, \mathbf{p}) = 1/[i\omega_m - \epsilon_{\mathbf{p}} + \mu]$. Summing over the intermediate frequency ω_m of the loop, obtain the following expression

$$\Pi(i\Omega_n, \mathbf{q}) = 2 \int \frac{d^3p}{(2\pi)^3} \frac{f(\epsilon_{\mathbf{p}+\mathbf{q}}) - f(\epsilon_{\mathbf{p}})}{i\Omega_n - \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{p}}}, \quad (5)$$

where $f(\epsilon)$ is the thermal Fermi distribution function.

Useful formula:

$$\sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)^2 + a^2} = \frac{\pi}{2a} \tanh \frac{\pi a}{2}. \quad (6)$$

(Can you derive this formula?)

4. [8 points] *Fluctuations of lattice displacements*

Let us consider the correlator of lattice displacements $\mathbf{u}(\mathbf{r}, t)$ at the same time t , but at different points in space \mathbf{r} :

$$C(\mathbf{r}) = \langle u_{\parallel}(\mathbf{r}) u_{\parallel}(0) \rangle, \quad (7)$$

where $u_{\parallel}(\mathbf{r}) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} (\mathbf{k} \cdot \mathbf{u}_{\mathbf{k}})/|\mathbf{k}|$ is the longitudinal component of displacement.

Express $C(\mathbf{r})$ in terms of the Matsubara Green function of phonons (see Problem 1 of HW 4). Separate the quantum contribution $C_0(\mathbf{r}) = \lim_{T \rightarrow 0} C(\mathbf{r})$ and the thermal contribution $C_T(\mathbf{r}) = C(\mathbf{r}) - C_0(\mathbf{r})$. When performing summation over the Matsubara frequencies, use the following formula:

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 + a^2} = \frac{\pi}{a} \coth(\pi a). \quad (8)$$

(Can you derive this formula?)

For the acoustic phonons, determine qualitatively how $C_0(\mathbf{r})$ and $C_T(\mathbf{r})$ behave at long distances r in the 1D, 2D, and 3D cases. Do they diverge? What can you say about the long-range order in 1D, 2D, and 3D crystals on the basis of these results?

5. [4 points] *Green function at a finite temperature*

The ordinary (not Matsubara) Green function at a finite temperature is defined by Eq. (36.12),

$$iG(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \langle \mathcal{T} \hat{\psi}(\mathbf{r}_1, t_1) \hat{\psi}^+(\mathbf{r}_2, t_2) \rangle, \quad (9)$$

where \mathcal{T} represents chronological ordering with respect to the ordinary (not Matsubara) time t , and the averaging is done with respect to the Gibbs distribution (36.1).

Using the expansion $\hat{\psi}(\mathbf{r}, t) = \sum_{\mathbf{p}} e^{i\mathbf{k}\cdot\mathbf{r} - i(\epsilon_{\mathbf{p}} - \mu)t} \hat{a}_{\mathbf{p}}$ and the definition (9), calculate $G(\omega, \mathbf{p})$ in the frequency-momentum representation for noninteracting particles. Show that

$$G(\omega, \mathbf{p}) = (1 \mp n_{\mathbf{p}})G^R(\omega, \mathbf{p}) + n_{\mathbf{p}}G^A(\omega, \mathbf{p}) = \frac{1 \mp n_{\mathbf{p}}}{\omega - \epsilon_{\mathbf{p}} + \mu + i0} + \frac{n_{\mathbf{p}}}{\omega - \epsilon_{\mathbf{p}} + \mu - i0}, \quad (10)$$

where the signs \mp refer to fermions and bosons, and $n_{\mathbf{p}}$ is the thermal distribution function for fermions or bosons.

Check whether Eq. (10) agrees with Eqs. (36.18) and (36.23).