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Methods of Statistical Physics
NFPL088, Wed 16:30, zoom/F155KFM

Problem Sheet 6

1 Spectrum of electron-hole pairs and the imaginary susceptibility

Show for which ω, q is the imaginary part of the susceptibility $\tilde{\chi}_0(\mathbf{q}, \omega)$ non-zero for a non-interacting homogeneous electron gas.

2 Negative absolute temperature

In this problem, you will show how absolute temperature can become negative. This phenomenon occurs in systems where the density of states can decrease with energy, *e.g.* few-level systems, magnets, excited atoms of a laser. In systems with a monotonously increasing density of states, like gasses, the negative absolute temperature does not occur.

To be specific, we consider N Ising spins, $s_i = \pm 1, i = 1 \dots N$, without interaction ($J = 0$) in an external magnetic field B. The energy is simply given by $H = -B \sum_i s_i = -BM$, where M is the magnetization, $M = \sum_i s_i$. Notice that in our notation the unit of B is the same as the unit of energy and M is dimensionless. The spins are isolated (not in contact with a heat reservoir).

The expression for the temperature follows straightforwardly from the first law of thermodynamics. For a constant B and N, it holds that the change of the energy is $\mathrm{d}E = T\mathrm{d}S$. From this relation, the temperature can be expressed:

$$T = \left(\frac{\partial S(E)}{\partial E} \right)^{-1}_{B,N=\text{const.}} \tag{1}$$

Because the spins are isolated, it is appropriate to use the microcanonical ensemble. The only parameter of the ensemble is energy, denoted here by E. The microstates are given by the orientation of the spins $\{s_i\}_{i=1}^N$ and we will label the microstates simply by the letter s. The energy of a given microstate is $E' = -B \sum_i s_i$. The probability of a microstate s will be denoted by p_s. In a microcanonical ensemble, p_s is zero, if $E \neq E'$ and nonzero (constant), if $E = E'$, or

$$p_s = \begin{cases} 1/g(E) & \text{if } E = -B \sum s_i \\ 0 & \text{if } E \neq -B \sum s_i \end{cases}$$

The constant $1/g(E)$ is easy to determine from a normalization condition. Because $\sum_s p_s = 1$, $g(E)$ is the mumber of microstates with energy E (check!).

Calculate the temperature $T(E)$ in these simple steps:

(a) In order to evaluate the Eq. (1), we first need an expression for the entropy, $S(E)$. It follows from the standard definition $S = -k\sum_s p_s \log(p_s)$. Show, that this expression simplifies to $S(E) = k\log[g(E)]$.

(b) The number of (micro)states with energy E, $g(E)$, is identical to the number of states with magnetization $M = -E/B$. This number was calculated in the Problem $\boxed{\mathbf{1}}$, Sheet 5, and it is $2^N w(M) = \frac{N!}{N_+!N_-!}$. Using this formula, express $g(E)$ as a function of E, B and N.

(c) Show, that $S(E)/k = \log(N!) - \log\left\{\left[\frac{1}{2}(N + E/B)\right]!\right\} - \log\left\{\left[\frac{1}{2}(N - E/B)\right]!\right\}$

(d) Evaluate the entropy at three important values: $E = 0$ and $E = \pm NB$. Think, why are these values special?

(e) Based on the latter three points, sketch a graph of $S(E)$.

(f) Now, sketch a graph of the temperature $T(E)$ based on your previous drawing of $S(E)$. Discuss your result.

(g) *Optional:* calculate $T(E)$ for small E using Stirling's formula $\log(n!) \approx n\log n - n$.

$\boxed{\mathbf{3}}$ Ornstein-Zernike behavior of spatial correlations

Consider a three-dimensional ferromagnet above the critical temperature. The non-local susceptibility is given by

$$\tilde{\chi}(k;T) = \frac{D^{-1}}{\xi^{-2}(T) + k^2}.$$

We label the lattice vector connecting sites 0 and m by $\mathbf{r}$. Your task is to evaluate the susceptibility in the real space,

$$\chi_{m0}(T) = \frac{1}{\Omega_{\mathrm{BZ}}}\int_{\mathrm{BZ}} \exp\left(-\mathrm{i}\mathbf{k}\cdot\mathbf{r}\right)\tilde{\chi}(k;T)\mathrm{d}^3\mathbf{k}, \qquad (2)$$

in the limit $\xi(T) \gg a$ and $|\mathbf{r}| \gg a$, following the steps below.

(a) From the lecture notes, recall the definitions of D and $\xi(T)$!

(b) In the first step, we extend the domain of integration to the whole reciprocal space. Try to justify this approximation. Inspect the integrand in Eq. (2) for $\mathbf{k}$ such, that $|\mathbf{k}| \gtrsim \frac{\pi}{a}$, and $\xi(T) \gg a$.

(c) Switch to the spherical coordinates and do the angular integrals!

(d) The remaining integral in k can be performed by complex contour integration. Before that, it has to be rewritten in a suitable form. Justify these steps:

- Notice, that the integral $\int_0^\infty$ is identical to $\int_{-\infty}^0$. Use this to extend the domain of integration to the entire real axis.
- Replace $\sin(kr)$ by $-\mathrm{i}\exp(\mathrm{i}kr)$.
- In the plane of complex k, the integration contour $k \in (-\infty, \infty)$ can be closed with a semicirlce of infinite radius in the upper half plane, where $\mathrm{Im}(k) > 0$.

(e) List the poles of the integrand in the complex k-plane. Hint: they are pure imaginary numbers.

(f) The resulting integral $\oint k e^{\mathrm{i}kr}/(\xi^{-2} + k^2)\mathrm{d}k$ can be evaluated easily by Cauchy's integral formula, because the contour encloses a single pole. You recover the result shown at the lecture, namely $\chi_{m0}(T) \propto \frac{\xi}{r}\exp\left(-r/\xi\right)$.