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1. Exercise of QFT for many-body systems

31.03.2011

1. Getting familiar with the Density of States *1*+2+2=1*+4 points*

Calculations of thermodynamic quantities, response functions and Feynman diagrams in QFT for condensed matter systems often require the evaluation of integrals or sums over all momenta **k** (typically over the first Brillouin Zone). An important simplification of these **k**-summations is possible, however, when the integrand $\mathcal{F}$ is depending **on the energy** only. In this case the integration/sum is best performed by using the energy ε as a variable. In the case of a cubic lattice of volume L^d in d dimensions we have for a given observable F:

$$F = \frac{1}{L^d}\sum_{\mathbf{k}} \mathcal{F}(\varepsilon_{\mathbf{k}}) = \frac{1}{(2\pi)^d}\frac{(2\pi)^d}{L^d}\sum_{\mathbf{k}} \mathcal{F}(\varepsilon_{\mathbf{k}}) \simeq \frac{1}{(2\pi)^d}\int d^dk\ \mathcal{F}(\varepsilon_{\mathbf{k}}) = \int d\varepsilon\, \mathcal{N}(\varepsilon)\, \mathcal{F}(\varepsilon) \qquad (1)$$

where $\mathcal{N}(\varepsilon)$, i.e. the so-called **D**ensity **o**f **S**tates (**DOS**), which can be defined via comparison between the different equalities as

$$\mathcal{N}(\varepsilon) = \frac{1}{L^d}\sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \text{ or, for the continuous case,} \qquad (2)$$

$$= \frac{1}{(2\pi)^d}\int d^dk\ \delta(\varepsilon - \varepsilon_{\mathbf{k}}). \qquad (3)$$

a) Calculate and plot the explicit expression for $\mathcal{N}(\varepsilon)$ for non-interacting particles of mass m in the continuous case (i.e., $\varepsilon_{\mathbf{k}} = \frac{\hbar^2k^2}{2m}$) in one, two and three dimensions. How do the corresponding Fermi surfaces look like in these cases?

b) Consider the following one-dimensional tight-binding Hamiltonian

$$H = -t\sum_{\langle i,j\rangle}\left[c^\dagger_{i,\sigma}c_{j,\sigma} + h.c.\right] \qquad (4)$$

with hopping ($t > 0$) restricted to next-neighboring sites, where $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ are the creation/annihilation operators for one electron with spin $\sigma = \uparrow, \downarrow$ at the position $x_i = i\ a$ with $i = 0, 1, ..., N$ and a being the lattice spacing. Assuming periodic boundary conditions ($x_0 = x_N$), compute the corresponding eigenenergies, e.g., using the following basis transformation (from real to momentum space)

$$c^\dagger_{k,\sigma} = \frac{1}{\sqrt{Na}}\sum_{x_i} \mathrm{e}^{-ikx_i}c^\dagger_{i,\sigma} \qquad (5)$$

for the fermionic operators.

c) How can one extend the results of **1b)** for arbitrary dimensions $d > 1$? Analyze explicitely the results obtained for $d = 2$, and try to plot (numerically) the DOSes $\mathcal{N}(\varepsilon)$ for the cases $d = 1, 2, 3$. Which are the most prominent features of theses DOS functions and at which energies ε they occur? How would the corresponding Fermi surfaces look like for the case $d = 1, 2$, e.g. if one has an average density of one electron per site (*half-filled system*)?

2. Screened and unscreened Coulomb Potentials *0.5*+1.5*=2* points*

a) From the integral representation of the delta function,

$$\delta(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \tag{6}$$

and the fact that the Coulomb potential $\phi(\mathbf{r}) = -e/r$ satisfies Poisson's equation,

$$-\nabla^2\phi(\mathbf{r}) = -4\pi e\delta(\mathbf{r}), \tag{7}$$

show that the electronic pair potential, $V(\mathbf{r}) = -e\phi(\mathbf{r}) = e^2/r$, can be written in the form

$$V(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\, V(\mathbf{k}), \tag{8}$$

where the Fourier transform $V(\mathbf{k})$ is given by

$$V(\mathbf{k}) = \frac{4\pi e^2}{k^2} \tag{9}$$

b) Show that the Fourier transf. of the screened Coulomb interaction $V_s(\mathbf{r}) = (e^2/r)\mathrm{e}^{-k_{TF}\,r}$ is

$$V_s(\mathbf{k}) = \frac{4\pi e^2}{k^2 + k_{TF}^2} \tag{10}$$

by substituting (10) into the Fourier integral

$$V_s(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\, V_s(\mathbf{k}), \tag{11}$$

and evaluating that integral in spherical coordinates (*Hint:* The radial integral is best done as a contour integral.). Finally, deduce from (10) that $V_s(\mathbf{r})$ satisfies

$$\left(-\nabla^2 + k_{TF}^2\right) V_s(\mathbf{r}) = 4\pi e^2 \delta(\mathbf{r}) \tag{12}$$

3. Calculations of the Lindhard function (I) *3 points*

Using the formula of first-order stationary perturbation theory,

$$|\psi_{\mathbf{k}}\rangle = |\psi^0_{\mathbf{k}}\rangle + \sum_{\mathbf{k}'} \frac{|\psi^0_{\mathbf{k}'}\rangle\langle\psi^0_{\mathbf{k}'}|V|\psi^0_{\mathbf{k}}\rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}} \tag{13}$$

and expressing the electronic charge density as

$$\rho(\mathbf{r}) = -e\sum_{\mathbf{k}} f_{\mathbf{k}} |\psi_{\mathbf{k}}(\mathbf{r})|^2 = \rho^0(\mathbf{r}) + \rho^{\mathrm{ind}}(\mathbf{r}) \tag{14}$$

(where $f_{\mathbf{k}}$ is the equilibrium Fermi distribution), show that the Fourier transform of the charge induced to first order in a total potential ϕ is given by

$$\rho^{\mathrm{ind}}(\mathbf{q}) = -e^2 \int \frac{d^3k}{4\pi^3} \frac{f_{\mathbf{k}-\frac{1}{2}\mathbf{q}} - f_{\mathbf{k}+\frac{1}{2}\mathbf{q}}}{\hbar^2(\mathbf{k}\cdot\mathbf{q}/m)} \phi(\mathbf{q}). \tag{15}$$

In which limit does the Lindhard screening approach the Thomas-Fermi one?

* Bonus points

Viel Spaß!