IFP
TU Wien

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4. Übung QFT für Vielteilchensysteme

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1. Getting familiar with the Density of States *2+3=5 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** $\varepsilon(\mathbf{k})$ 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:

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

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

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

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

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

b) Consider the energy dispersion $\varepsilon(\mathbf{k}) = -2t\sum_{i=1}^{d}\cos(k_i a)$ derived in the last exercise for the d-dimensional Hubbard-model. Try to plot (numerically) the DOS $\mathcal{N}(\varepsilon)$ for the cases $d = 1, 2, 3$. Which are the most prominent features of these 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*)?
For further information see also: A. Georges, G. Kotliar, et.al., Rev.Mod.Phys. 68 (Appendix A).

2. Calculations of the <u>Lindhard</u> function (I) *2+3=5 points*

In perturbation theory the state of a system, at first order in the perturbation, is given by:

$$|\psi_{\mathbf{k}}\rangle = |\psi^0_{\mathbf{k}}\rangle + \sum_{\mathbf{k}'} \frac{|\psi^0_{\mathbf{k}'}\rangle\langle\psi^0_{\mathbf{k}'}|V|\psi^0_{\mathbf{k}}\rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}}. \tag{4}$$

a) Suppose that the perturbation V is generated by an external[1] charge distribution:

$$\langle\mathbf{r}|V|\mathbf{r}'\rangle = -e\delta(\mathbf{r} - \mathbf{r}')\phi(\mathbf{r}), \tag{5}$$

and, assuming that the wave functions $\psi(\mathbf{r}) = \langle\mathbf{r}|\psi^0_{\mathbf{k}}\rangle$ of the unperturbed system are plain waves, express the matrix element $\langle\psi^0_{\mathbf{k}}|V|\psi^0_{\mathbf{k}+\mathbf{q}}\rangle$ in terms of the Fourier transform $\phi(\mathbf{q})$ of the electrostatic potential.

b) Express the distribution of the electronic charge density as:

$$\rho(\mathbf{r}) = -e \sum_{\mathbf{k}} f_{\mathbf{k}} |\psi_{\mathbf{k}}(\mathbf{r})|^2 = \rho^0 + \rho^{\text{ind}}(\mathbf{r}) \tag{6}$$

(where $f_{\mathbf{k}}$ is the equilibrium Fermi distribution), ρ^0 is the density of the unperturbed system and $\rho^{\text{ind}}(\mathbf{r})$ is the variation of the density at *first order* in the perturbation. Show that the Fourier transform of the charge induced to first order in the potential ϕ is given by

$$\rho^{\text{ind}}(\mathbf{q}) = -e^2 \int \frac{d^3k}{4\pi^3} \frac{f_{\mathbf{k}-\frac{1}{2}\mathbf{q}} - f_{\mathbf{k}+\frac{1}{2}\mathbf{q}}}{\hbar^2(\mathbf{k}\cdot\mathbf{q}/m)} \phi(\mathbf{q}). \tag{7}$$

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

[1] The perturbation is generated by an *external* distribution of charge, therefore it can be treated here as a *one particle* potential.

3. Screened and unscreened Coulomb Potentials *0 points*

(Additional exercise for the Thomas-Fermi model which will not be graded, but just discussed by the tutor.)

a) From the integral representation of the delta function,

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

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

$$-\nabla^2\phi(\mathbf{r}) = -4\pi e\delta(\mathbf{r}), \tag{9}$$

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

$$V(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\, V(\mathbf{k}), \tag{10}$$

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

$$V(\mathbf{k}) = \frac{4\pi e^2}{k^2} \tag{11}$$

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

$$V_s(\mathbf{k}) = \frac{4\pi e^2}{k^2 + k_{TF}^2} \tag{12}$$

by substituting (12) into the Fourier integral

$$V_s(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\, V_s(\mathbf{k}), \tag{13}$$

and evaluating that integral in spherical coordinates (*Hint:* The radial integral is best done as a contour integral.). Finally, deduce from (12) that $V_s(\mathbf{r})$ satisfies

$$\left(-\nabla^2 + k_{TF}^2\right) V_s(\mathbf{r}) = 4\pi e^2\delta(\mathbf{r}) \tag{14}$$