Assignments to Condensed Matter Theory I
Sheet 11

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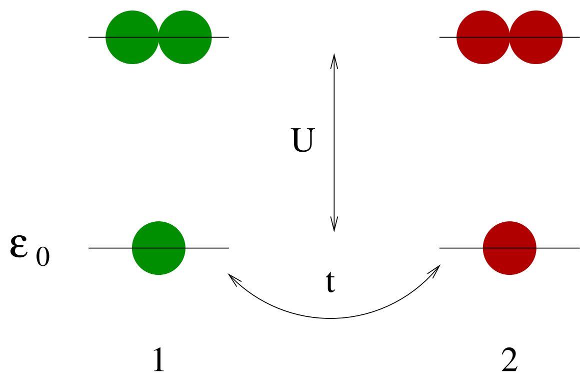
sheet online: http://www-MCG.uni-R.de/teaching/

Problem set: Electron-Electron Interaction (II)

11.1. Double site Hubbard model

The Hubbard Hamiltonian for a two site system reads explicitly:

$$H = \epsilon_0 \left(c^\dagger_{1\uparrow} c_{1\uparrow} + c^\dagger_{1\downarrow} c_{1\downarrow} + c^\dagger_{2\uparrow} c_{2\uparrow} + c^\dagger_{2\downarrow} c_{2\downarrow} \right) + t \left(c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{2\downarrow} c_{1\downarrow} + c^\dagger_{2\uparrow} c_{1\uparrow} + c^\dagger_{1\downarrow} c_{2\downarrow} \right)$$
$$+ U \left(c^\dagger_{1\uparrow} c_{1\uparrow} c^\dagger_{1\downarrow} c_{1\downarrow} + c^\dagger_{2\uparrow} c_{2\uparrow} c^\dagger_{2\downarrow} c_{2\downarrow} \right)$$



(a) Calculate the two particle eigenenergies analytically. Treat the case of parallel and antiparallel spin separately. Plot the results as a function of U/t.
Hint: For the antiparallel case consider the basis of the corresponding Hilbert space:

$$c^\dagger_{1\uparrow} c^\dagger_{1\downarrow}|0\rangle,\ c^\dagger_{2\uparrow} c^\dagger_{2\downarrow}|0\rangle,\ c^\dagger_{1\uparrow} c^\dagger_{2\downarrow}|0\rangle,\ c^\dagger_{2\uparrow} c^\dagger_{1\downarrow}|0\rangle$$

Calculate the matrix elements of H in this basis and diagonalize the resulting 4×4 matrix.

(b) Calculate the ground state in the Hartree-Fock approximation and compare it with the exact result of point (a).

11.2. Homogeneous electron gas in the Hartree-Fock approximation

Show that the following identities hold by transforming the sums over $\mathbf{k}'$ and k into integrals and evaluate them.

(a)

$$\frac{1}{V}\sum_{\substack{\mathbf{k}' \\ (k'\leq k_\mathrm{F})}}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2}=\frac{1}{2\pi^2}k_\mathrm{F}\left[\frac{1}{2}+\frac{1-(k/k_\mathrm{F})^2}{4(k/k_\mathrm{F})}\ln\left|\frac{1+k/k_\mathrm{F}}{1-k/k_\mathrm{F}}\right|\right]$$

(b)

$$\sum_{k<k_\mathrm{F}}\frac{k_\mathrm{F}^2-k^2}{kk_\mathrm{F}}\ln\left|\frac{k+k_\mathrm{F}}{k-k_\mathrm{F}}\right|=\frac{V}{6\pi^2}k_\mathrm{F}^3.$$

11.3. [Kür] Thomas Fermi limit in atomic physics

Let us consider an atom with a positively charged nucleus with a charge $Z|e|$ (where e is the electronic charge taken with the sign) and its surrounding electron shells. In the Hartree limit the potential felt by each electron at position $\mathbf{r}$ is given by the expression:

$$V(\mathbf{r})=\int d\mathbf{r}\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}n(\mathbf{r})-\frac{Ze^2}{r} \tag{1}$$

where $n(\mathbf{r})$ is the density of electrons. In the Thomas-Fermi approximation one can assume that the potential is varying so slowly that can be considered constant around a given point $\mathbf{r}$. Then it is allowed to introduce a local homogemeous electron gas for the region around the point $\mathbf{r}$.

(a) Justify that, from the previous assumption, it follows that

$$n(\mathbf{r})=\frac{[2m(\epsilon_\mathrm{F}-V(\mathbf{r}))]^{3/2}}{3\pi^2}$$

where ϵ_F is the energy of the highest occupied energy level.

(b) Justify that for a neutral atom $\epsilon_\mathrm{F}=0$.

(c) Prove that Eq. (1) is equivalent to the Poisson equation and derive from that and using the result of point (b) the Thomas-Fermi equation:

$$-\frac{3\pi}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V(r)}{\partial r}\right)=4e^2[2m(\epsilon_\mathrm{F}-V(\mathbf{r}))]^{3/2} \tag{2}$$

Hint: The charge distribution and the associated potential can be considered spherically symmetric.

(d) Show that, by introducing the Bohr radius a_0 as length unit,

$$V(r)=-\frac{Ze^2}{r}\Phi(x),\ r=Z^{-1/3}bx,\ b=\frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3}a_0,\ a_0=\frac{1}{me^2}$$

Eq. (2) becomes the following differential equation for the dimensionless potential $\Phi(x)$:

$$\frac{\mathrm{d}^2}{\mathrm{d}^2x}\Phi(x)=x^{-1/2}\Phi^{3/2}(x) \tag{3}$$

with the boundary conditions

$$\Phi(0) = 1, \lim_{x\to\infty} \Phi(x) = 0 \tag{4}$$

`Note:` We have assumed $\hbar = 1$ and $4\pi\varepsilon_0 = 1$.

(e) Solve Eq. (3) numerically and plot the functions $\Phi(x)$, $V(r)$ and $4\pi r^2 n(r)$.