Assignments to Condensed Matter Theory I

Sheet 11

G. Cuniberti (Phy 4.1.29) Room H35
A. Donarini (Phy 3.1.24) Mon 17.07 (h 10.15)

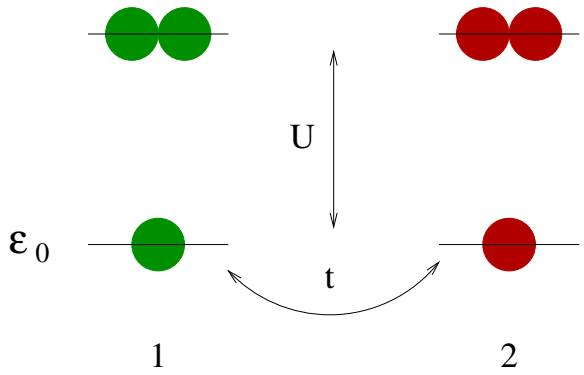
sheet online: `http://www-MCG.uni-R.de/teaching/`

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)

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

(b)

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

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

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

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

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

(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:

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

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 $4\pi r^2 n(r)$.

SOLUTIONS OF THE EXERCISES FOR THE SHEET 11 OF QTKM1

11.1 Double site Hubbard model

$$H = \varepsilon_0 \left(c^\dagger_{1\uparrow} c_{1\uparrow} + c^\dagger_{1\downarrow} c_{1\downarrow} + c^\dagger_{2\uparrow} c_{2\uparrow} + c^\dagger_{2\downarrow} c_{2\downarrow} \right) +$$

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

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

a) Two particle with parallel spin can be inserted in the system only in the form:

$$c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} |0\rangle \quad \text{or} \quad c^\dagger_{1\downarrow} c^\dagger_{2\downarrow} |0\rangle$$

Note that we assume the order of the particle to be

$$1\uparrow \; 2\uparrow \; 1\downarrow \; 2\downarrow$$

PARALLEL

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

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

$$H|+,+\rangle = 2\varepsilon_0 |+,+\rangle$$

$$H|-,-\rangle = 2\varepsilon_0 |-,-\rangle$$

ANTIPARALLEL

The space of the antiparallel case is spanned by the 4 vectors:

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

$$|+,-\rangle \equiv c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} |0\rangle \,, \quad |-,+\rangle \equiv c^\dagger_{2\uparrow} c^\dagger_{1\downarrow} |0\rangle$$

$$H|2,0\rangle = 2\varepsilon_0|2,0\rangle + t\left(|+,-\rangle + |-,+\rangle\right) + U|2,0\rangle$$

$$H|0,2\rangle = 2\varepsilon_0|0,2\rangle + t\left(|+,-\rangle + |-,+\rangle\right) + U|0,2\rangle$$

$$H|+,-\rangle = 2\varepsilon_0|+,-\rangle + t\left(|0,2\rangle + |2,0\rangle\right)$$

$$H|-,+\rangle = 2\varepsilon_0|-,+\rangle + t\left(|0,2\rangle + |2,0\rangle\right)$$

We choose the basis with the order:

$$|2,0\rangle\ ,\ |0,2\rangle\ ;\ |+,-\rangle\ ,\ |-,+\rangle$$

The matrix representation of H reads:

$$H = \begin{bmatrix} 2\varepsilon_0+U & 0 & t & t \\ 0 & 2\varepsilon_0+U & t & t \\ t & t & 2\varepsilon_0 & 0 \\ t & t & 0 & 2\varepsilon_0 \end{bmatrix}$$

$\det|H - \lambda\mathbb{1}| = 0$ is the eq. in λ to find the eigenvalues. We define $\mu = \lambda - 2\varepsilon_0$

$$0 = \det\begin{vmatrix} U-\mu & 0 & t & t \\ 0 & U-\mu & t & t \\ t & t & -\mu & 0 \\ t & t & 0 & -\mu \end{vmatrix} = (U-\mu)\det\begin{vmatrix} U-\mu & t & t \\ t & -\mu & 0 \\ t & 0 & -\mu \end{vmatrix} + t\det\begin{vmatrix} 0 & U-\mu & t \\ t & t & 0 \\ t & t & -\mu \end{vmatrix}$$

$$- t\det\begin{vmatrix} 0 & U-\mu & t \\ t & t & -\mu \\ t & t & 0 \end{vmatrix} =$$

$$= (U-\mu)\left[(U-\mu)\mu^2 + 2\mu t^2\right] + 2t\left[\cancel{t^3} \cancel{-t^3} + \mu t(U-\mu)\right] =$$

$$= (U-\mu)\left[(U-\mu)\mu^2 + 4\mu t^2\right] = (U-\mu)\mu\left[(U-\mu)\mu + 4t^2\right] = \mu(U-\mu)\left[-\mu^2 + U\mu + 4t^2\right]$$

$$\mu_1 = 0 \qquad \lambda_1 = 2\varepsilon_0$$
$$\mu_2 = U \qquad \lambda_2 = 2\varepsilon_0 + U$$

$$\mu_{3,4} = \frac{+U \pm \sqrt{U^2 + 16t^2}}{2} \qquad \lambda_{3,4} = 2\varepsilon_0 + \frac{U}{2}\left(1 \pm \sqrt{1 + \frac{16t^2}{U^2}}\right)$$

The ground state energy is given in any case by

$$\lambda_3 = 2\varepsilon_0 + \frac{U}{2}\left(1 - \sqrt{1 + \frac{16t^2}{U^2}}\right)$$

If $t \ll U$

$$\lambda_{3,4} \cong 2\varepsilon_0 - \frac{4t^2}{U} \;,\; 2\varepsilon_0 + U + \frac{t^2}{U}$$

If $t \gg U$

$$\lambda_{3,4} \cong 2\varepsilon_0 + \frac{U}{2}\left(1 \pm \frac{4|t|}{U}\sqrt{1 + \frac{U^2}{16t^2}}\right)$$

$$= 2\varepsilon_0 + 2|t|\left(\frac{U}{4|t|} \pm \sqrt{1 + \frac{U^2}{16t^2}}\right) \sim 2\varepsilon_0 \pm 2|t| + \frac{U}{2}$$

b) The ground state in Hartree-Fock approximation can be calculated starting with:

$$H_{HF} = \varepsilon_0 \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} + t \sum_\sigma \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma}\right)$$
$$+ U\left(\bar{n}_{1\uparrow}\, c^\dagger_{1\downarrow} c_{1\downarrow} + c^\dagger_{1\uparrow} c_{1\uparrow}\, \bar{n}_{1\downarrow} - \bar{n}_{1\uparrow}\bar{n}_{1\downarrow} + \right.$$
$$\left. + \bar{n}_{2\uparrow}\, c^\dagger_{2\downarrow} c_{2\downarrow} + c^\dagger_{2\uparrow} c_{2\uparrow}\, \bar{n}_{2\downarrow} - \bar{n}_{2\uparrow}\bar{n}_{2\downarrow}\right)$$

Now we need to calculate $\bar{n}_{1\uparrow}\ \bar{n}_{1\downarrow}\ \bar{n}_{2\uparrow}\ \bar{n}_{2\downarrow}$ in a 2 particle system. (we are already neglecting $\uparrow\downarrow$ coherences)

Since we also want to treat only the case $S_z = 0$, we assume $\bar{n}_{1\uparrow} = \bar{n}_{1\downarrow}$. Since the Hamiltonian is invariant under the transformation $1 \leftrightarrow 2$ we also take $\bar{n}_{1\uparrow} = \bar{n}_{2\uparrow} = \bar{n}_{2\downarrow} = \bar{n}_{1\downarrow} = n$. Since

$$\sum_{i\sigma} \bar{n}_{i\sigma} = 2 = 4n \qquad n = \frac{1}{2}$$

$$H_{HF} = \varepsilon_0 \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} + t \sum_{\sigma} \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right) +$$

$$+ \frac{U}{2} \sum_{i\sigma} c^\dagger_{\sigma} c_{i\sigma} - \frac{U}{2} .$$

This Hamiltonian is easily diagonalized and the eigenvalues are

$\varepsilon_0 + \frac{U}{2} + t$ $\quad 2\times$ for the $\sigma = \uparrow$ and $\downarrow$

$\varepsilon_0 + \frac{U}{2} - t$ $\quad 2\times$

$\Rightarrow$ the ground state energy in HF :

$$\varepsilon_g = 2\varepsilon_0 + U - \frac{U}{2} + 2t = 2\varepsilon_0 + \frac{U}{2} + 2t$$

Let us compare this result with the exact ($t < 0$)

$$\cancel{2\varepsilon_0} + \frac{U}{2} + 2t \leq \cancel{2\varepsilon_0} + \frac{U}{2} - \frac{U}{2}\sqrt{1 + \frac{16t^2}{U^2}}$$

$$2|t| \geq \frac{U}{2}\sqrt{1 + \frac{16t^2}{U^2}}$$

$$4|t|^2 \geq \frac{U^2}{4}\left(1 + \frac{16t^2}{U^2}\right) \qquad 0 \geq \frac{U^2}{4}$$

Hartree-Fock over-estimate the ground state and is better the smaller the interaction.

11.2 Homogeneous electron gas in the Hartree-Fock approx.

a)

$$\frac{1}{V}\sum_{\substack{\bar{k}'\\ k'<k_F}} \frac{1}{|\bar{k}-\bar{k}'|^2} = \frac{1}{V}\int_{k'<k_F} \frac{d\bar{k}'}{(2\pi)^3}\cdot L_x L_y L_z \frac{1}{|\bar{k}-\bar{k}'|^2} =$$

$$= \frac{1}{(2\pi)^3}\int_0^{k_F} dk' \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\, k'^2 \sin\theta \frac{1}{k'^2+k^2-2kk'\cos\theta} =$$

$$= \frac{1}{4\pi^2}\int_0^{k_F} dk' \int_{-1}^{1} d\alpha \frac{k'^2}{k'^2+k^2-2kk'\alpha} = \frac{-1}{4\pi^2}\int_0^{k_F} dk' \frac{k'^2}{2kk'}\left(\ln|k'^2+k^2-\alpha 2kk'|\right)\Big|_{-1}^{1}$$

$$= \frac{1}{4\pi^2}\int_0^{k_F} dk' \frac{k'}{2k} \ln\left|\frac{(k'+k)^2}{(k'-k)^2}\right| = \frac{1}{4\pi^2 k}\int_0^{k_F} dk' \left[k' \ln|k'+k| - k'\ln|k'-k|\right]$$

$$= \frac{1}{4\pi^2 k}\left\{\left(\frac{k'^2}{2}\ln|k'+k|\right)\Big|_0^{k_F} - \int_0^{k_F}\frac{k'^2}{2}\cdot\frac{1}{k'+k} - \left(\frac{k'^2}{2}\ln|k'-k|\right)\Big|_0^{k_F} + \int_0^{k_F}\frac{k'^2}{2}\frac{1}{k'-k}\right\} =$$

$$= \frac{1}{4\pi^2 k}\left\{\frac{k'^2-k^2}{2}\ln|k'+k| - \frac{k'^2}{4} + \frac{kk'}{2} - \frac{k'^2-k^2}{2}\ln|k'-k| + \frac{k'^2}{4} + \frac{kk'}{2}\right\}\Big|_0^{k_F}$$

$$= \frac{1}{4\pi^2 k}\left(\frac{k_F^2-k^2}{2}\ln\left|\frac{k_F+k}{k_F-k}\right| + kk_F\right) = \frac{1}{2\pi^2}k_F\left(\frac{1}{2} + \frac{1-(k/k_F)^2}{4(k/k_F)}\ln\left|\frac{1+k/k_F}{1-k/k_F}\right|\right).$$

b)

$$\sum_{k<k_F}\frac{k_F^2-k^2}{kk_F}\ln\left|\frac{k+k_F}{k-k_F}\right| = \frac{V}{(2\pi)^3}\int_0^{k_F} dk \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\, k^2\sin\theta \frac{k_F^2-k^2}{kk_F}\ln\left|\frac{k+k_F}{k-k_F}\right|$$

$$= \frac{V}{2\pi^2}\int_0^{k_F} dk \frac{k(k_F^2-k^2)}{k_F}\ln\left|\frac{k+k_F}{k-k_F}\right| = \frac{V}{2\pi^2}\int_0^{k_F} dk \frac{1}{2k_F} k^2(k_F^2-k^2)\cdot\left(\frac{1}{k+k_F} - \frac{1}{k-k_F}\right)$$

$$= \frac{V}{6\pi^2}k_F^3$$

11.3 Thomas Fermi limit in atomic physics

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

a) $n(\bar{r}) = \dfrac{[2m(\varepsilon_F - V(\bar{r}))]^{3/2}}{3\pi^2}$. The reason is that one can assume a local Fermi energy $\varepsilon_F(r) = \varepsilon_F - V(\bar{r})$

Now the local density is obtained in a canonical way:

$$N = \sum_{k\sigma} n_F(\varepsilon_k) = 2V \int_0^{k_F} \frac{d\bar{k}}{(2\pi)^3} =$$

$$= \frac{1}{\pi^2} V \frac{1}{3} k_F^3 = \frac{V}{3\pi^2} \left(\frac{\hbar^2 k_F^2}{2m} \cdot \frac{2m}{\hbar^2} \right)^{3/2} = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar^2} \varepsilon_F \right)^{3/2} \qquad \hbar = 1$$

$$n = \frac{(2m\varepsilon_F)^{3/2}}{3\pi^2}$$

b) The Fermi energy ε_F is uniquely defined all over the space. Far from the nucleus $n(r) \to 0$ since this is the electronic density and, at the same time $V(r) \to 0$ since the charge of the nucleus compensate the electronic charge. From a) it follows:

$$\boxed{\varepsilon_F = 0}$$

c)

It is emph to take the Laplacian of (1)

$$\nabla_r^2 V(r) = \int dr' \nabla_r^2 \frac{e^2}{|r-r'|} n(r') - \nabla_r^2 \frac{Ze^2}{r}$$

$$= -\int dr' 4\pi \delta(r-r') e^2 n(r') - 4\pi Z e^2 \delta(r)$$

$$= -4\pi \left[e^2 n(r) - Ze^2 \delta(r) \right]$$

$$V(r) = e\phi(r) \Rightarrow -\nabla^2 \phi(r) = 4\pi \left[e n(r) - Ze\, \delta(r) \right]$$

Thus for $r \neq 0$

$$-\nabla^2 \phi(r) = 4\pi e\, n(r)$$

$$-\nabla^2 V(r) = -\left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right] e\, \phi(r) = 4\pi e^2 \frac{\left[2m(\varepsilon_F - V(r)) \right]^{3/2}}{3\pi^2}$$

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

d) $V(r) = -\frac{Ze^2}{r} \phi(x) \qquad r = z^{-1/3} b x \qquad b = \frac{1}{2} \left(\frac{3\pi}{4} \right)^{2/3} a_0 \qquad a_0 = \frac{1}{me^2}$

$\boxed{\varepsilon_F = 0}$

$$+\frac{3\pi}{x^2} \frac{z^{2/3}}{b^2} \frac{\partial}{\partial x} \left(x^2 \frac{\partial}{\partial x} \frac{z a^2}{x b} z^{1/3} \phi(x) \right) = +4 a^2 (2m)^{3/2} \frac{z^{3/2} e^3}{b^{3/2} x^{3/2}} z^{1/2} \phi^{3/2}(x)$$

$$\frac{3\pi z^2}{b^3} \frac{1}{x^2} \frac{\partial}{\partial x} x^2 \frac{\partial}{\partial x} \frac{1}{x} \phi(x) = \frac{4 e^3 (2m)^{3/2} z^2}{b^{3/2}} \frac{1}{x^{3/2}} \phi^{3/2}(x)$$

$b^{3/2}$

$$b^{3/2} = \frac{1}{2^{3/2}} \frac{3\pi}{4} a_0^{3/2} = \frac{3\pi}{4} \cdot \frac{1}{(2me^2)^{3/2}}$$

$$\frac{1}{x^2} \frac{\partial}{\partial x}\left[x^2 \frac{\partial}{\partial x}\left(\frac{1}{x}\phi(x)\right)\right] = \frac{1}{x^{3/2}} \phi^{3/2}(x)$$

$$\frac{1}{x^2} \frac{\partial}{\partial x}\left[x^2 \left(\left(-\frac{1}{x^2}\right)\phi(x) + \frac{1}{x}\frac{\partial}{\partial x}\phi(x)\right)\right] =$$

$$= \frac{1}{x^2} \frac{\partial}{\partial x}\left[-\phi(x) + x\frac{\partial}{\partial x}\phi(x)\right] = x\frac{\partial^2}{\partial x^2}\phi(x) = \frac{1}{x^{3/2}}\phi^{3/2}(x)$$

$$\boxed{\frac{d^2}{dx^2}\phi(x) = x^{-1/2}\phi^{3/2}(x)}$$

$\lim_{x\to 0} \phi(x) = \lim_{r\to\infty} -\frac{r}{ze^2}V(r) = 1$ since $n(\vec{r}')$ is not contributing

$\lim_{x\to\infty} \phi(x) = \lim_{r\to+\infty} -\frac{r}{ze^2}V(r) = 0$ since $V(r) = 0$ outside the atom.

e)