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Theorie zu Magnetismus, Supraleitung und Elektronische Korrelation in Festkörpern

Sommersemester 2019

Blatt 2

(Abgabe: 30.04.2019)

Aufgabe 1 (**Derivation of the Hartree Equations from the Variational Principle**) (3=1+2 Punkte)

Consider the many-body Hamiltonian H,

$$\hat{H} = \sum_i \left(-\frac{\hbar^2}{2m}\hat{k}_i^2 + V(\hat{\vec{r}})\right) + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\hat{\vec{r}}_i - \hat{\vec{r}}_j|}$$

$$\langle r_1 \dots r_N|\hat{H}|r'_1 \dots r'_N\rangle = \left(\sum_i \left(-\frac{\hbar^2}{2m}\vec{\nabla}_i^2 + V(\vec{r})\right) + \frac{1}{2}\sum_{i\neq j} u(\vec{r}_i,\vec{r}_j)\right)\prod_{i=1}^{N}\delta(r_i - r'_i),$$

$$= \left(\sum_i \hat{h}_i(\vec{r}_i) + \frac{1}{2}\sum_{i\neq j} u(\vec{r}_i,\vec{r}_j)\right)\prod_{i=1}^{N}\delta(r_i - r'_i),$$

acting on the N-particle wave function $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$ (we omit the spin index as our Hamiltonian does not have any spin dependent terms). Within the Hartree approximation, the eigenstates of H are *not* antisymmetrized and determined by setting

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2)\dots\varphi_N(\vec{r}_N)$$

and then minimizing the expectation value $\langle\Psi|\hat{H}|\Psi\rangle$.

a) Show that

$$\begin{aligned}\langle\Psi|\hat{H}|\Psi\rangle &= \sum_i \int d\vec{r}\; \varphi_i^*(\vec{r})\; \hat{h}(\vec{r})\; \varphi_i(\vec{r}) \\ &+ \frac{1}{2}\sum_{i\neq j}\int d\vec{r} d\vec{r}\,'\; u(\vec{r},\vec{r}\,')\; |\varphi_i(\vec{r})|^2 |\varphi_j(\vec{r}\,')|^2,\end{aligned}$$

provided that all the $\varphi_i(\vec{r})$ satisfy the normalization condition $\int d\vec{r}\, |\varphi_i(\vec{r})|^2 = 1$.

b) With the constraint of normalization for each $\varphi_i(\vec{r})$ expressed with a Lagrange multiplier ε_i and with $\delta\varphi_i(\vec{r})$ and $\delta\varphi_i^*(\vec{r})$ taken as independent variations, the stationary condition for $|\Psi\rangle$ is given as

$$\frac{\delta}{\delta\varphi_n^*(\vec{r})}\left[\langle\Psi|H|\Psi\rangle - \varepsilon_n\left(\int d\vec{r}\,'\; |\varphi_n(\vec{r}\,')|^2 - 1\right)\right] = 0.$$

Show that this stationary condition leads directly to the Hartree equations

$$\left[h(\vec{r}) + \sum_j \int d\vec{r}\,'\; u(\vec{r},\vec{r}\,')\; |\varphi_j(\vec{r}\,')|^2\right]\varphi_n(\vec{r}) = \varepsilon_n\varphi_n(\vec{r}).$$

(*Hint*: Make use of $\dfrac{\delta}{\delta\phi(x)}\displaystyle\int dy\; f(y)\phi(y) = f(x)$.)

Aufgabe 2 (**Hartree-Fock energy of the Homogeneous Electron Gas for the Coulomb Potential**) (7 Punkte)

In the homogeneous electron gas, the total charge [external charge sources $V(\vec{r})$ + electron charge $V^{\text{Hartree}}(\vec{r})$] at any spacial position is neutral, *i.e.*,

$$V(\vec{r}) = V^{\text{Hartree}}(\vec{r}).$$

In this case, the Hartree-Fock equations reduce to

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\varphi_i(\vec{r}) + \sum_j \int d\vec{r}\,' \; \varphi_j^*(\vec{r}\,')\frac{e^2}{|\vec{r}-\vec{r}\,'|}\varphi_i(\vec{r}\,')\varphi_j(\vec{r}) = \varepsilon_i\varphi_i(\vec{r}). \tag{1}$$

The solutions to these equations are plane waves $\varphi_{i\to\vec{k}}(\vec{r}) = \frac{1}{\sqrt{v}}e^{i\vec{k}\cdot\vec{r}}$ ($v :=$ volume), while the eigenenergies can be calculated by transforming Eq. (1) into the reciprocal space

$$\frac{\hbar^2 k^2}{2m}\varphi_{\vec{k}}(\vec{r}) - \int_{|\vec{q}|<k_F} \frac{d\vec{q}}{(2\pi)^3}\frac{4\pi e^2}{|\vec{k}-\vec{q}|^2}\varphi_{\vec{k}}(\vec{r}) = \varepsilon_{\vec{k}}\varphi_{\vec{k}}(\vec{r})$$

Show that the Hartree-Fock correction with respect to the non-interacting electron gas energy $\frac{\hbar^2 k^2}{2m}$ is given by

$$-\int_{|\vec{q}|<k_F} \frac{d\vec{q}}{(2\pi)^3}\frac{4\pi e^2}{|\vec{k}-\vec{q}|^2} = -\frac{e^2}{\pi}k_F\left(1+\frac{1-x^2}{2x}\ln\left|\frac{1+x}{1-x}\right|\right), \quad x = \frac{k}{k_F}.$$

Hint: Perform integration in the spherical coordinates. You can use the identities

$$\int \ln|x| \;\mathrm{d}x = x\ln|x| - x$$

$$\int x\ln|x| \;\mathrm{d}x = \frac{x^2}{2}(\ln|x| - \frac{1}{2})$$