Pauliprinzip & viele Elektronen

Schrödingergl. für $\Psi(\vec{r}_1 s_1; \vec{r}_2 s_2; \ldots; \vec{r}_N s_N)$ lösen.

(Terme für E_{kin}, E_{kern-e}, E_{ee}) hoffnungslos

effektive Einteilchen S.Gl mit eff. e-e-Potential U_{el}
(mean field → s. FP)

$$U_{ek}(\vec{r}) = -e \int d\vec{r}\,' \rho(\vec{r}\,') \frac{1}{|\vec{r} - \vec{r}\,'|}$$ für e bei $\vec{r}$

$$\text{mit } \rho(\vec{r}) = -e \sum_i |\psi_i(\vec{r})|^2$$

Hartree-Gleichung

Es fehlt das Pauliprinzip!

Deshalb statt einfachem Produktansatz

$$\psi_1(\vec{r}_1,\vec{s}_1)\cdot\psi_2(\vec{r}_2,\vec{s}_2)\cdot\ldots\cdot\psi_N(\vec{r}_N,\vec{s}_N)$$

eine Slaterdeterminante als Ansatz:

$$\psi(\vec{r}_1,\vec{s}_1,\ldots) = \begin{vmatrix} \psi_1(\vec{r}_1,\vec{s}_1) & \psi_1(\vec{r}_2,\vec{s}_2) & \cdots & \psi_1(\vec{r}_N,\vec{s}_N) \\ \psi_2(\vec{r}_1,\vec{s}_1) & & & \\ \vdots & & & \vdots \\ \psi_N(\vec{r}_1,\vec{s}_1) & & & \psi_N(\vec{r}_N,\vec{s}_N) \end{vmatrix}$$

$\Rightarrow$ Hartree-Fock-Gleichung

o.k. für Atome & kleine Moleküle

für FK i.A. nicht lösbar.

außer für FEG.

Resultat: $\frac{E}{N} = \frac{e^2}{2a_0}\left[\underbrace{\frac{3}{5}(k_F a_0)^2}_{\text{mittl. } E_{kin}} - \underbrace{\frac{3}{2\pi} k_F a_0}_{E_x}\right]$

(!! HF überschätzt Austausch, weil Abschirmung fehlt

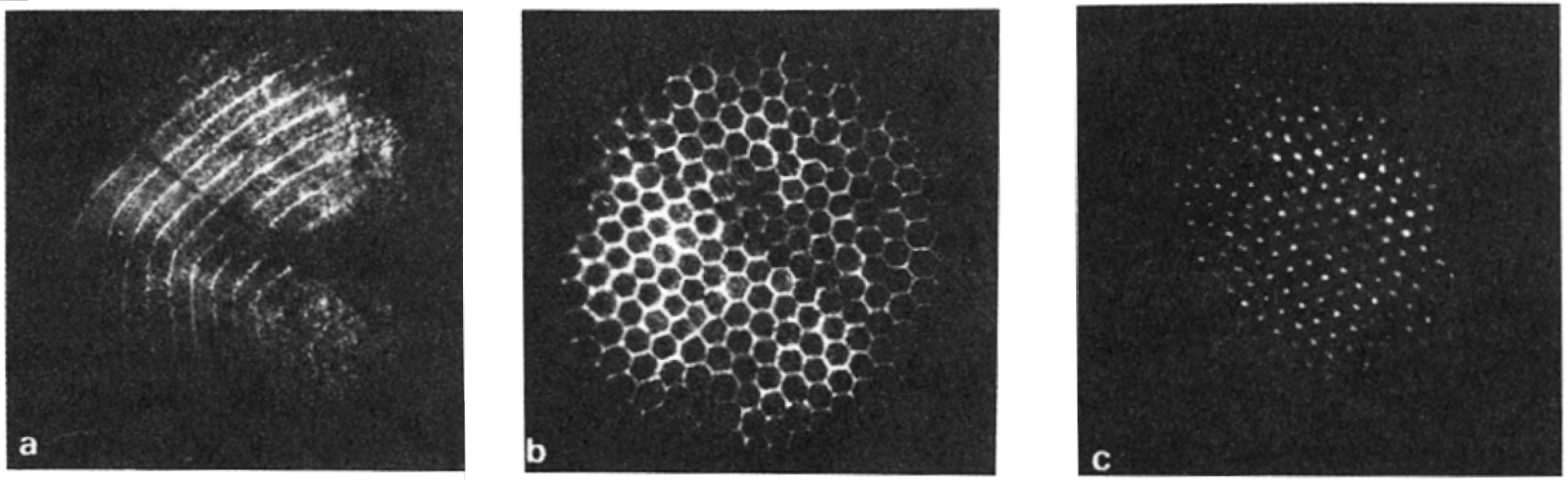
- bei geringen Dichten: Wignerkristall)

E. Wigner, On the Interaction of Electrons in Metals, Phys. Rev. **46**, 1002 (1934)

If the electrons had no kinetic energy, they would settle in configurations which correspond to the absolute minima of the potential energy.
These are closed-packed lattice configurations, with energies very near to that of the bodycentered lattice.

Wie verringert man E_{kin}?

Elektronen auf flüssigem He



aus: Electrons at the Surface of Quantum Systems,
P. Leiderer, J. Low Temp. Phys. 87(1992)

Fig. 11. Formation of a dimple lattice on a ^{4}He surface ($T = 3.5$ K) charged with electrons from above. The pictures show the surface deformation approximately 2s(a) and 6s((b) and (c)) after the field had been increased to E_c. The image plane in (a) and (b) was chosen such that convex deformations of the surface, corresponding to local maxima, appear bright; in (c) bright areas correspond to local minima (i.e. the center of the dimples). The distance between adjacent rows of dimples is close to the wavelength $2\pi a$ of the soft ripplon, 0.24 cm in this case.

aktueller: 2DEGs in (Al)GaAs-Schichtsystemen:

n mit Potentialen einstellbar