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Electron Liquids: Ground State

I. INTERACTIONS IN A SYSTEM OF BROAD-BAND ITINERANT ELECTRONS

A. Introduction remarks

$$H_{el\ liquid} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}\sum_{i,j} V_{Coulomb}(r_i - r_j)$$
$$+\ \ interaction\ \ with\ \ background; \tag{1}$$

in semiconductors $m \to m_b$ and $e^2 \to e^2/\epsilon$.

Unlike the ordinary gas, the interaction of electrons can be neglected only for high density, while at low or even intermediate densities it is a system of strongly interacting particles.

What is a possibility of the ferromagnetism in the liquid of itinerant electrons?

B. Physical meaning of $r_s = r_0/a_B$

A dimensionless parameter where r_0 is the radius of an artificial sphere "belonging" to one electron in the electron liquid, and

$a_B = \hbar^2/me^2 \approx 0.529$Å$= 5.29nm.$

In the case of semiconductors one should use the band mass m_b and e^2/ϵ. It can easily be that $a_B^* \gg a_B$.   Rydberg

$E(p_F)$ as a typical kinetic energy. What is p_F (defined as a position of a jump in the occupation numbers) in the interacting system?

The Luttinger theorem: the jump in the occupation numbers occurs along the Fermi surface in such a way that it confines the same volume in the momentum space as if the fermion particles are free from interactions

$$N = 2\sum_{p<p_F} 1 =_{|3D} 2\frac{4\pi p_F^3}{3(2\pi\hbar)^3}V = V\frac{p_F^3}{3\pi^2\hbar^3}. \tag{2}$$

$$\left.\frac{p_F r_0}{\hbar}\right|_{3D} = \left(\frac{9\pi}{4}\right)^{1/3} \approx 1.9. \tag{3}$$

$$E_{\text{F-free;3D}} = \frac{p_F^2}{2m} = \left(\frac{9\pi}{4}\right)^{2/3} \frac{\hbar^2}{2mr_0^2} = \left(\frac{9\pi}{4}\right)^{2/3} \frac{1}{r_s^2} \left(\frac{me^4}{2\hbar^2}\right). \tag{4}$$

In terms of $\left(\frac{me^4}{2\hbar^2}\right) = 1$ Ry,

$$E_{\text{F-free;3D}} = \frac{3.68}{r_s^2} \text{ Ry}. \tag{5}$$

$$E_C = \frac{e^2}{\epsilon r_0} = \frac{e^2}{r_s a_0} = \frac{2}{r_s} \text{ Ry}. \tag{6}$$

Combination $e^2/\hbar v_F$ (more precisely $e^2/\epsilon\hbar v_F$):

$$\frac{e^2}{\epsilon\hbar v_F} = \frac{e^2}{\epsilon a_B r_s} \frac{r_0}{\hbar v_F} = \frac{2r_0}{\hbar v_F} \frac{\text{Ry}}{r_s}. \tag{7}$$

$$\left.\frac{e^2}{\epsilon\hbar v_F}\right|_{3D} = \frac{r_s}{1.9}. \tag{8}$$

If $r_s \lesssim 1$, the Coulomb interaction is effectively small and can be treated perturbatively.

In the opposite case of large r_s (low electron density) both the kinetic energy and the energy of e-e interaction decrease, but the kinetic energy does it faster.

In the region of moderately large r_s a quantitative treatment of the effects of the Coulomb interaction is problematic.

In $2D$ one has to substitute 1.9 by $\sqrt{2}$:

$$\frac{p_F r_0}{\hbar} = \sqrt{2}; \qquad E_F = \frac{2}{r_s^2} \text{ Ry}; \tag{9}$$

$$\frac{e^2}{\epsilon\hbar v_F} = \frac{r_s}{\sqrt{2}}; \qquad \frac{E_C}{E_F} = r_s. \tag{10}$$

The energy of the bound states in $2D$:

$E_n = -4/(2n+1)^2$ Ry where $n = 0, 1, 2...$

C.   what deviation of r_s from unity says

Typical value of E_F in simple metals is about few eV. Let it be $5eV$ (this should be compared with 1 Rydberg = 13.6eV).

$mc^2 \approx 0.5meV$ (by comparison with c, one can easily evaluate that in metals $v_F \sim 10^3 km/\sec \sim 10^{-2}c$). Therefore, $\frac{e^2}{\hbar v_F} = \frac{e^2}{\hbar c}\frac{c}{v_F} \approx 5^{1/2}\frac{100}{137} \approx 1.5$. We estimate that $r_s \approx 3$.

In simple metals $2 \lesssim r_s \lesssim 5.5$. Why it is systematically > 1?

In a hydrogen molecule H_2

$r_s = \frac{0.74}{2 \cdot 0.53} \approx 0.7$.

A substantial deviation from $r_s \sim 1$ indicates that there should be an additional component of non-Coulomb origin which shifts the equilibrium from a point where $r_s \sim 1$.

The strongly interacting electrons with r_s systematically exceeding 1, and an almost free Fermi surface, are in fact the consequence of the *pseudo-potential* physics

D.   Charged Background and Electro-neutrality

$$H = \sum \epsilon_p a^\dagger_{p\sigma} a_{p\sigma} + \frac{1}{2V} \sum_{pqk;\sigma,\sigma'} V_C(k) a^\dagger_{p+k,\sigma} a^\dagger_{q-k,\sigma'} a_{q\sigma'} a_{p\sigma} + background \tag{11}$$

the $3D$ Fourier transform of the Coulomb interaction is equal to $V_C(k) = 4\pi e^2/\epsilon k^2$; note that together with factor $1/V$ the interaction term in the Hamiltonian has a correct dimension of energy

The $2D$ Fourier transform of the $3D$ Coulomb interaction yields $V_C(k) = 2\pi e^2/\epsilon \mid k \mid$.

[Electrons are confined within a $2D$ plane, but the electric field does not. Therefore, the Poisson equation should be solved in $3D$. That is how the $2D$ transform of the $3D$ Coulomb interaction appears. One can look on it as $4\pi e^2 \int dk_z/\epsilon(k^2+k_z^2)$, where the k_z- integration fixes the z-coordinate in the $3D$ Coulomb interaction $e^2/\sqrt{r^2 + z^2}$ within the plane $z = 0$.]

The singularity at in $V_C(k)$ $k \to 0$ leads to a serious complication when one naively averages the interaction term

$$E_{Hartree} = \frac{1}{2V} \sum_{pqk;\sigma,\sigma'} V_C(k) \left\langle a^\dagger_{p+k,\sigma} a^\dagger_{q-k,\sigma'} a_{q\sigma'} a_{p\sigma} \right\rangle \Rightarrow \tag{12}$$

$$\Longrightarrow \frac{1}{2V} \sum_{pqk;\sigma,\sigma'} V_C(k) \left\langle a^\dagger_{p+k,\sigma} a_{p\sigma} \right\rangle \left\langle a^\dagger_{q-k,\sigma'} a_{q\sigma'} \right\rangle \underset{k=0}{=} \frac{1}{2V} \sum_{p,q;\sigma,\sigma'} V_C(k = 0) n_{p\sigma} n_{q\sigma'}.$$

Small-k terms yield $Q^2/2C$ with a capacitance $C \sim L$.

Instead of Q, one has to consider the charge difference $(Q - Q_{bgr})$ and correspondingly the total energy of charges is $(Q - Q_{bgr})^2/2C$

The condition of electro-neutrality:

$\lim(Q - Q_{bgr})/V \to 0$

For a mesoscopic system of a nano-scale size the effect introduced by a finite charge leads to an important phenomenon, which is called the Coulomb blockade.

For low dimensional electrons confined within a conducting channel of a nanometer scale width one can vary the *density* of electrons in wide limits.

When the charging energy is ignored, one simply excludes the $k = 0$ Fourier-components from all Coulomb interactions. Then, the sum over momenta in the *e-e* interaction is written as $\sum_{pqk \neq 0} V_C(k) a^\dagger_{p+k,\sigma} a^\dagger_{q-k,\sigma'} a_{q\sigma'} a_{p\sigma}$.

E. Correlations: (i) Exchange interaction

$$\Psi_{\text{Hartree−Fock}} = a^\dagger_N a^\dagger_{N-1} \cdots a^\dagger_j \cdots a^\dagger_1 \mid empty \quad vacuum\rangle, \tag{13}$$

where the states $1, ...j...N-1, N$ cover all the wave functions with the momenta $p < p_F$. The kinetic energy per one particle

$$E_{\text{av}} = \frac{3}{5} E_{\text{F}} = \frac{2.21}{r_s^2} \text{ Ry.} \tag{14}$$

The Fock term represents the exchange contribution into the energy of interaction:

$$E_{Fock} = \frac{1}{2V} \sum_{pqk;\sigma,\sigma'} V_C(k) \left\langle a^\dagger_{p+k,\sigma} a^\dagger_{q-k,\sigma'} a_{q\sigma'} a_{p\sigma} \right\rangle \Rightarrow \tag{15}$$

$$-\frac{1}{2V} \sum_{pqk;\sigma,\sigma'} V_C(k) \left\langle a^\dagger_{p+k,\sigma} a_{q\sigma'} \right\rangle \left\langle a^\dagger_{q-k,\sigma'} a_{p\sigma} \right\rangle_{\overline{q=p+k;\sigma=\sigma'}} -\frac{1}{2V} \sum_{p,k;\sigma} V_C(k) n_{p+k\sigma} n_{p\sigma}.$$

Unlike the Hartree term, there is only one summation over spins in the Fock term.

a pair of electrons exchange their states: $(p + k)\sigma \rightleftarrows p\sigma$

In the case of contact interaction $V(q) = const$, the interaction contributions within the same spin species are cancelled out.

The Green's functions presented in the Hartree-Fock diagrams were substituted by the occupation numbers. It works only for a Green's function at equal times: $G(t_1, t_2)_{t_1 \to t_2}$. Coulomb interaction is instantaneous, and forces the time difference to be zero.

A note about the volume factors: Each summation when substituted by the integration yields a factor of volume. So, eventually one gets an expression that is explicitly proportional to the volume, as it should be for an extensive property. In many articles this volume factor is omitted, assuming $V = 1$.

In $3D$ the Fock term yields the exchange energy per particle equal to

$$E_{\text{exch};3D} = -\frac{1}{2NV} \sum_{p,k;\sigma} V_C(k=0) n_{p+k\sigma} n_{p\sigma} = -\frac{0.916}{r_s} \text{ Ry.} \tag{16}$$

The Hartree-Fock energy:

$$E_{\text{HF};3D} = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right) \text{ Ry.} \tag{17}$$

F.   Correlations: (ii) non-zero spin polarization

In the discussed case the Hartree term is absent, and therefore in the Hartree-Fock approximation the two spin species are disconnected;

$E_{HF} = E_{HF}(p_F)$, but for the fully polarized state $p_{F\uparrow} = 2^{1/3} p_F$.

The difference in energy of the fully polarized states versus the unpolarized phase per one electron:

$$\Delta E_{HF;3D} = \frac{1.30}{r_s^2} - \frac{0.238}{r_s}. \tag{18}$$

It becomes negative when $r_s \geq 5.46$.

The $2D$ electron gas (liquid) in heterostructures can be made very dilute. The energy difference between the unpolarized and polarized state in the Hartree-Fock approximation is equal to

$$\Delta E_{HF;2D} = \frac{1}{r_s^2} - \frac{1.2(\sqrt{2}-1)}{r_s} \text{ Ry.} \tag{19}$$

It changes its sign at $r_s \approx 2$.

The output of the measurements of the spin susceptibility: no transition into the ferromagnetic state so far. What is wrong?

G. Correlation functions (following the book of Pines)

The instantaneous density-density correlation function $\rho_2(\mathbf{r}^1, \mathbf{r}^2)$:

$$\rho_2(\mathbf{r}^1, \mathbf{r}^2) = \left\langle \Psi \left| \sum_{a,b} \delta(\mathbf{r}^1 - \mathbf{r}_a) \delta(\mathbf{r}^2 - \mathbf{r}_b) \right| \Psi \right\rangle \equiv \tag{20}$$

$$\int \cdots \int \Psi^*\{\mathbf{r}_i\}_N \left\{ \sum_{a,b} \delta(\mathbf{r}^1 - \mathbf{r}_a) \delta(\mathbf{r}^2 - \mathbf{r}_b) \right\} \Psi\{\mathbf{r}_i\}_N d^N\mathbf{r}_i,$$

This function carries the information about the instantaneous (i.e., a snapshot photo) distribution of the electron density in the ground state. For the translational invariant state, $\rho_2(\mathbf{r}^1, \mathbf{r}^2)$ depends on the difference $\mathbf{r} = \mathbf{r}^1 - \mathbf{r}^2$:

$$\rho_2(\mathbf{r}) = \frac{1}{V} \left\langle \Psi^* \left| \sum_{a,b} \delta(\mathbf{r} - \mathbf{r}_a + \mathbf{r}_b) \right| \Psi \right\rangle. \tag{21}$$

It is common to introduce a function $p(\mathbf{r})$, such that

$$\rho_2(\mathbf{r}^1, \mathbf{r}^2) = \widetilde{\rho}\, p(\mathbf{r}^1 - \mathbf{r}^2), \tag{22}$$

where $\widetilde{\rho} = N/V$ is the average density. Obviously, at large distances $p(r \to \infty) = \widetilde{\rho} = N/V$. The function $p(\mathbf{r})$ determines the structure form factor:

$$S(\mathbf{k}) = \int p(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} d\mathbf{r}. \tag{23}$$

With the use of

$$p(\mathbf{r}) = \frac{1}{N} \left\langle \Psi^* \left| \sum_{a,b} \delta(\mathbf{r} - \mathbf{r_a} + \mathbf{r_b}) \right| \Psi \right\rangle, \tag{24}$$

one gets,

$$S(\mathbf{k}) = \frac{1}{N} \left\langle \Psi^* \left| \sum_{a,b} e^{-i\mathbf{k}(\mathbf{r_a} - \mathbf{r_b})} \right| \Psi \right\rangle =$$

$$= \frac{1}{N} \left\langle \Psi^* \left| \sum_b e^{i\mathbf{k}\mathbf{r_b}} \sum_a e^{-i\mathbf{k}\mathbf{r_a}} \right| \Psi \right\rangle = \frac{1}{N} \left\langle \Psi^* \left| \rho^\dagger(k)\rho(k) \right| \Psi \right\rangle. \tag{25}$$

A term which describes a trivial correlation of a particle with itself, i.e., when $a = b$ can be single out

$$
\begin{aligned}
p(\mathbf{r}) &= \delta(\mathbf{r})_{|_{a=b}} + \frac{1}{N}\langle\Psi|\sum_{a\neq b}\delta(\mathbf{r} - \mathbf{r_a} + \mathbf{r_b})|\Psi\rangle \\
&= \delta(\mathbf{r}) + \frac{(N-1)}{V}g(\mathbf{r}).
\end{aligned}
\tag{26}
$$

$g(r)$ is the binary correlation function characterizing the probability to find two different particles on a distance $\mathbf{r}$ from each other.

$$
g(\mathbf{r}) = \frac{V}{N(N-1)}\langle\Psi|\sum_{a\neq b}\delta(\mathbf{r} - \mathbf{r_a} + \mathbf{r_b})|\Psi\rangle.
\tag{27}
$$

If there is no correlations $g(r) = 1$. At large distances particles do not know about each other, and move without correlations: $g(r \to \infty) = 1$.

Technically it is more convenient to calculate $g(r)$ via $S(k)$:

$$
S(k) = 1 + \frac{N-1}{V}g(k); \quad g(r) = \frac{1}{N-1}\sum_k(S(k) - 1)e^{i\mathbf{kr}}.
\tag{28}
$$

The density operator

$$
\rho(k) = \sum_{p,\sigma}a^\dagger_{(p+k)\sigma}a_{p\sigma}.
\tag{29}
$$

The structure form factor:

$$
\begin{aligned}
S(k) &= \frac{1}{N}\langle\Psi|\sum_{p,q;\sigma,\widetilde{\sigma}}a^\dagger_{(p+k)\sigma}a_{p\sigma}a^\dagger_{(q-k)\widetilde{\sigma}}a_{q\widetilde{\sigma}}|\Psi\rangle = \\
&\quad 1 + \frac{1}{N}\langle\Psi|\sum_{p,q;\sigma,\widetilde{\sigma}}a^\dagger_{(p+k)\sigma}a^\dagger_{(q-k)\widetilde{\sigma}}a_{q\widetilde{\sigma}}a_{p\sigma}|\Psi\rangle.
\end{aligned}
\tag{30}
$$

In the Hartree approximation only the average within the same pairs is permitted. For $k \neq 0$ the second term vanishes, and

$$
S_{\mathrm{H}}(k) = 1 + (N-1)\delta_{0,k}.
\tag{31}
$$

Correspondingly,

$$
g(r) = \frac{1}{N-1}\sum[S(k) - 1]e^{ikr} \stackrel{\text{Hartree}}{=} \frac{1}{N-1}\sum_{k=0}e^{ikr}(N-1)\delta_{0,k} = 1.
\tag{32}
$$

No correlations, as it should be in the Hartree approximation.

The exchange term:

$$S_{\mathrm{HF}}(k) = 1 + \frac{1}{N}\langle\Psi_{\mathrm{HF}}|\sum a^{\dagger}_{p+k,\sigma}a^{\dagger}_{q-k,\widetilde{\sigma}}a_{q,\widetilde{\sigma}}a_{p,\sigma}|\Psi_{\mathrm{HF}}\rangle =$$

$$1 + (N-1)\delta_{0,k} - \frac{1}{N}\sum_{p,\sigma}n_{p+k,\sigma}n_{p\sigma} \qquad for \quad k\neq 0 \quad only.$$

For $k > 2k_F$ the sum in the last term vanishes, and $S_{\mathrm{HF}}(k > 2k_F) = 1$. This expression can be rearranged in a way that the limitation $k \neq 0$ can be omitted:

$$S_{\mathrm{HF}}(k) \stackrel{\mathrm{rearrangement}}{=} N\delta_{0,k} + \frac{1}{N}\sum_{p,\sigma}n_{p\sigma}(1 - n_{p+k,\sigma}). \tag{33}$$

(At $T = 0$, $n_p(1 - n_{p+k}) \rightarrow 0$ when $k \rightarrow 0$ as the same state cannot be empty and occupied at the same time.) Finally,

$$S_{\mathrm{HF;3D}}(k) = N\delta_{0,k} + \frac{3}{4}\frac{k}{k_F} - \frac{1}{16}\frac{k^3}{k_F^3}; \ k < 2k_F \tag{34}$$

$$= 1 \qquad\qquad k > 2k_F. \tag{35}$$

The function $S_{\mathrm{HF}}(k)$ is non-analytic at $k = 2k_F$.

For the binary correlation function one gets:

$$g_{\mathrm{HF}}(r) = 1 - \frac{9}{2}\left[\frac{\sin(k_F r) - k_F r\cos(k_F r)}{k_F^3 r^3}\right]^2. \tag{36}$$

The obtained $2k_F$-oscillation dependence in $g(r)$ is a poor cousin of the famous Friedel oscillations induced in the density of conducting electrons by a point defect.

It is natural to split $g_{\mathrm{HF}}(r)$ in two pieces

$$g_{\mathrm{HF}}(r) = \frac{1}{2} + g_{\mathrm{HF}}^{\uparrow\uparrow}(r) \tag{37}$$

The Pauli principle provides a strong correlation effect for electrons with parallel spins at small distances, $g_{\mathrm{HF}}^{\uparrow\uparrow}(r \rightarrow 0) = 0$.

Since the correlations keep electrons with the parallel spin projections away from each other, the curve $g(r)$ should go below $g_{\mathrm{HF}}(r)$ at small r.

The decoration of Slater determinant by the correlation factors:

$$\Psi_{\mathrm{corr}} = \chi_{\mathrm{slater}}\prod_{a\neq b}f(r_a - r_b). \tag{38}$$

The correlation factor can be chosen such that

$$f(r) \rightarrow 0; \text{ when } r \rightarrow 0$$
$$\rightarrow 1; \text{ when } r \rightarrow \infty$$

The energy, which is gained in the *e-e* interaction (! interaction, but not the total energy) due to the correlations

$$E_{e-e} = \frac{e^2}{2} \int \widetilde{\rho} \left[\frac{g(r) - 1}{r} \right] dr. \tag{39}$$

The difference $(1 - g(r))$ sometimes is called the correlation hole.

In the Hartree approximation, $g = 1$, and $E_{e-e} = 0$. For the unpolarized Hatree-Fock this expression yields a term $-0.916/r_s$ Ry in E_{HF}. Some energy is gained in the energy of the *e-e* interaction, but not as much as for the spin polarized state where $g(r \rightarrow 0) = 0$.

By modifying the wave function with the correlation factors the situation with the interaction energy can be made almost as good as in the spin polarized case but paying not so much in the kinetic energy.

[Confusion because of semantics:

the term "correlations" is commonly used in two sense: as an effect that keeps electrons away from each other and also as a modification of the wave function of the unpolarized state compared to the Hartree-Fock solution.]

At large r_s, the energies of different states are such that

$$E_{\mathrm{HF-unpol}} > E_{\mathrm{HF-pol}} > E_{\mathrm{pol}}^{\mathrm{f-corr}} > E_{\mathrm{unpol}}^{\mathrm{f-corr}}. \tag{40}$$

Compared to $E_{\mathrm{HF-unpol}}$, the energy $E_{\mathrm{unpol}}^{\mathrm{f-corr}}$ acquires a relatively big gain in the *e-e* interaction, $\Delta E_{\mathrm{unpol-ee}}^{\mathrm{f-corr}} < 0$, and a moderate loss in the kinetic energy $\Delta E_{\mathrm{unpol-kin}}^{\mathrm{f-corr}} > 0$. For $E_{\mathrm{pol}}^{\mathrm{f-corr}}$ both corrections are small. In result, $E_{\mathrm{unpol}}^{\mathrm{f-corr}}$ may become the most favorable state.

H.   Wigner crystal at $r_s \gg 1$

Arranging electrons in a lattice is an effective way to increase the negative value of the correlated energy.

The electrostatic energy (per electron) of the lattice $E_{\text{Lattice}} = \frac{1}{2N}\sum_{a,b}\frac{e^2}{|\mathbf{R}_a - \mathbf{R}_b|} = \frac{1}{2}\sum_{a\neq 0}\frac{e^2}{R_a}$. Together with the compensating background,

$$E_{\text{ch arg e}} = \frac{1}{2}\sum_{a\neq 0}\frac{e^2}{R_a} - \frac{1}{2}\int \widetilde{\rho}\frac{e^2}{r}dr; \tag{41}$$

$$E_{\text{ch arg e;3D}} = -1.792/r_s \text{ Ry}. \tag{42}$$

(Should be compared with $-0.916/r_s$ obtained for unpolarized Hartree-Fock, or $-1.15/r_s$ the polarized one.)

Copying the nature: in the "atomic units" redefined for ions, should stand the ion mass M instead of m. Ions in the metals are in the extreme dilute conditions, $\varrho_s = (M/m)r_s \ggg 1$. Liquid of charged fermions have to copy ions when it is very dilute. Wigner himself used a term "inverted alkali metal".

Quantum effects in the Wigner crystal: an electron moves in the potential well created by the electrostatic interaction with other electrons. As a trial wave function, one can take the Slater determinant from the set of wave functions:

$$\Phi_\alpha(x_i) = \phi(r_i - R_\alpha)\chi_\sigma(\xi_i). \tag{43}$$

where ϕ are the oscillatory wave functions $\phi(\delta r) \sim \exp(-\frac{1}{2}(\delta r/\zeta)^2)$ centered around points R_α of the Wigner crystal; ζ is the variation parameter.

The accurate calculation yields $E_{\text{zpm}} = 2.66/r_s^{3/2}$ Ry. The obtained estimate of the energy of electrons in the Wigner crystal state yields

$$E_{\text{Wigner}} = E_{\text{ch arg e}} + E_{\text{zpm}} = -1.792/r_s \text{ Ry} + 2.66/r_s^{3/2} \text{ Ry}. \tag{44}$$

[What stands in E_{zpm} is $3/2$ of the Debye frequency of electrons. Let us compare it with the Debye frequency of ions. One should first substitute r_s with ϱ_s and introduce M in the fake Rydberg. Then, to express everything back in the atomic units: $\omega_{\text{D}} \sim \left(\frac{m}{M}\right)^{1/2} r_s^{-3/2}$ Ry $\sim 10^3 K$, as it should be.]

I. The hierarchy of energies in the electron liquid at different r_s

At small r_s: 1) kinetic energy $>$ 2) Coulomb energy $>$ 3) and 4) correlation corrections to the e-e interaction and the kinetic energy. The Coulomb energy here is given in the form of the exchange interaction, i.e., the Fock term. The correlation energy appears because of modification of the wave function, e.g., by the f-factors.

At large r_s (both for liquid and Wigner crystal): 1) the interaction of electrons $>$ 2) kinetic energy $>$ 3) correlation energy treated as corrections to the zero-point motion $>$ 4) exchange energy.

The dominant term in the Coulomb interaction has been evaluated as the Hartree term for the Wigner crystal. In the liquid phase, it stems from the correlations in the e-e interaction. Exchange

is given as the ring exchange of few electrons. In the Wigner crystal it is responsible for spin arrangement.

The interpolation formula for the correlation energy in the unpolarized liquid at intermediate values r_s (Pines, following Wigner):

$$E_{\text{correlation}} = -\frac{0.88}{r_s + b} \text{ Ry}. \tag{45}$$

(In the old days the correlation energy was always defined as the deviation of the total energy of the system from the E_{HF}.)

Note that $\frac{-0.916}{r_s} + \frac{-0.88}{r_s} = \frac{-1.8}{r_s}$.

The constant b was chosen from the Wigner's estimate of the energy of the electron liquid at $r_s \lesssim 1$.

In $2D$,

$$E_{\text{Wigner}} = -2.21/r_s \text{ Ry} + 1.63/r_s^{3/2} \text{ Ry}. \tag{46}$$

The Monte Carlo calculations show that in $D = 2$ the Wigner crystal becomes a ground state only at $r_s \gtrsim 35$.

Should we be surprised that electron liquid remains stable up to r_s as large as 35?

II.   ELECTRONS IN QUANTIZED MAGNETIC FIELD

A.   Remarks for orientation

In the given $B_\perp$, the particle capacity of one Landau level is equal to $N_{\text{LL}} = \phi/\phi_0$, where $\phi = SB$ is the total flux piercing the area S and the quantum flux $\phi_0 = 2\pi\hbar/e$.

The filing factor is equal to $\nu \equiv N/N_{\text{LL}} = N\frac{\phi_0}{\phi} = \frac{2\pi\hbar}{eB}\widetilde{\rho}$, where $\widetilde{\rho}$ is the particle density N/S of $2D$ electrons.

Strong magnetic field radically changes the rule of the game.

What are the natural units for electrons in the quantized magnetic field?

For orientation: cyclotron frequency $\omega_{\text{c}} = \frac{\hbar eB}{mc}$, the cyclotron radius $l = (\hbar c/eB)^{1/2}$, and $E_{\text{F}}(B = 0) = \frac{\nu}{2}\omega_{\text{c}}$. The ratio of l to the typical distance between the electrons, $r_0 = 1/(\pi\widetilde{\rho})^{1/2}$:

$$l/r_0 = \left(\frac{\pi\hbar c\widetilde{\rho}}{eB}\right)^{1/2} = \left(\frac{\nu}{2}\right)^{1/2}. \tag{47}$$

The ratio $E_{\text{C}}/\omega_{\text{c}} = (\nu/2)(E_{\text{C}}/E_F) = (\nu/2)r_s$. It will be assumed that

$$(\nu/2)r_s \ll 1. \tag{48}$$

The minimal problem:

electrons confined within the lowest Landau level;

admixture with higher Landau levels is ignored.

Also for simplicity it will be assumed that the electrons are fully spin polarized by the magnetic field.

The uncertainty of the order l of the two coordinates of a particle, $[x, y] \sim l^2$.

Similarity with the Wigner crystal:

The main energy scale is the energy of the Coulomb interaction on the inter-particle distance.

Besides that, there are corrections induced by the quantum fluctuations: $E_{\mathrm{zpm}} \sim E_C (\delta r / r_0)^2$.

Difference: the energy E_{zpm} is controlled by the magnetic field.

The estimate of the relative strength of quantum fluctuations gives $E_{\mathrm{zpm}}/E_C \sim (l/r_0)^2 = \nu/2$.

In the Wigner crystal $(\delta r / r_0)^2 \sim 1/r_s^{1/2}$.

$\nu \ll 1$ acts as $1/r_s^{1/2}$

The energy of electrons at the lowest Landau level is defined in units e^2/l. Omitting $\omega_{\mathrm{c}}/2$, the main term in the energy per particle is $\sim \nu^{1/2}$, while the leading correction is about $\nu^{3/2}$.

B. Laughlin state

What kind of wave functions are in play?

The wave function of an electron projected on the lowest Landau level is an arbitrary polynomial of $z = (x + iy)/l$ multiplied by the exponential factor $\exp(-|z|^2/4l^2)$.

(The exponential factor is the same for all states and people keep it in mind but not always write.)

The Slater determinant for the case when the filling factor $\nu = 1$:

$$\psi_{\mathrm{HF}}^{\nu=1} = \begin{Vmatrix} \phi_1(z_1), \cdots, \phi_j(z_1), \cdots, \phi_N(z_1) \\ \phi_1(z_2), \cdots, \phi_j(z_2), \cdots, \phi_N(z_2) \\ \cdots, \cdots, \cdots, \cdots, \cdots \\ \phi_1(z_N), \cdots, \phi_j(z_N), \cdots, \phi_N(z_N) \end{Vmatrix} \tag{49}$$

Functions ϕ_α will be taken within the polynomials with the powers of z not exceeding N.

The answer is

$$\psi_{\text{HF}}^{\nu=1}(z_i, \cdots, z_N) = \prod_{i \neq j}(z_i - z_j) \exp\left(-\sum_i \frac{|z_i^2|}{4}\right) \tag{50}$$

This state has been constructed following the Hartree-Fock recipe. In fact, for $\nu = 1$ this is the only possible solution.

$\nu = 1/3, \implies$ lot of degeneracy is remained.

The ground state of a quantum liquid should be featureless:

$$\psi_{\text{L}}^{\nu=1/3}(z_i, \cdots, z_N) = \prod_{i \neq j}(z_i - z_j)^3 \exp\left(-\sum_i \frac{|z_i^2|}{4}\right) \tag{51}$$

Polynomial character of the wave functions controls the wave function both on the short and long(!) distances. Like in the case of $\nu = 1$, (almost) all resources are exhausted.

Laughlin's wave functions wins the competition in energy with the Wigner crystal from $\nu = 1/3$ to $\approx 1/5$.

C. Laughlin' liquid versus Wigner' crystal at small ν (following the discussion of Lam and Girvin (1984)).

The Hartree-Fock wave function of the Wigner crystal (i.e., the uncorrelated Wigner crystal)

$$\Psi_{\text{WC}}^{\text{uncorr}}(z_i, \cdots, z_N) = \text{antisymmetrized} \prod_{\alpha=1}^{N} \phi_\alpha(z_i). \tag{52}$$

$\phi_\alpha(z_i)$ is a single-particle state located near the site R_α of a probe lattice, which eventually is determined as triangular.

Function $\phi_\alpha(z_i)$ is a product of two terms (K.Maki and X. Zotos (1983)):

$$\phi_\alpha(z_i) = (2\pi)^{-1/2} \exp[-\frac{1}{4}|z_i - R_\alpha|^2 - -\frac{1}{4}(z_i^* R_\alpha - z_i R_\alpha^*)]. \tag{53}$$

The remarkable feature of this function:

(i) it is constructed within the basis of the lowest Landau level,

(ii) the exponential location of a particle near the site R_α is not spoiled by the second factor

$(z_i^* R_\alpha - z_i R_\alpha^*)^* = -(z_i^* R_\alpha - z_i R_\alpha^*)$

Energy of the Hartree-Fock state of the Wigner crystal ($\nu < 1/2$) is

$$E_{\text{WC}}^{\text{uncorr}} = -0.782133\nu^{1/2} + 0.2823\nu^{3/2} + 0.18\nu^{5/2}(r) - 1.41e^{-2.07/\nu}. \tag{54}$$

Here, $-0.782133\nu^{1/2}$ is the classic energy of the Coulomb energy. The last term describes exchange.

The correlated Wigner crystal state disfavors fluctuations corresponding to the longitudinal modes. It gives a slightly improved energy of the zero-point oscillations: $0.2410\nu^{3/2} + 0.16\nu^{5/2}$.

Comparison with the energy of the Laughlin function. The interpolation formula for filling factors $\nu = 1/(2m + 1)$:

$$E_{\text{L}} = -0.782133\nu^{1/2} + 0.165\nu^{1.24} + ... \tag{55}$$

!!!The Laughlin liquid state reproduces the classic energy of the Coulomb crystal!!!

The uncorrelated Hartree-Fock state beats the Laughlin liquid only around $\nu \sim 1/9$. For the correlated one it happens at $\nu \sim 1/6$.

Surprisingly, $\nu \sim 1/6$ and $r_s \sim 35$ correspond to each other.

III.   STABILITY OF THE ELECTRON LIQUID

A.   Melting of a $2D$ quantum liquid

Why $r_s \sim 35$ may, is a surprisingly low number.

The Lindemann criteria for melting is $\left\langle \delta r^2 \right\rangle^{1/2} / a \sim 0.15$.

In the Wigner crystal $\left\langle \delta r^2 \right\rangle^{1/2} / r_0 \sim 1/r_s^{1/4}$ or $(\nu/2)^{1/2}$ in the case of the magnetic field. This corresponds to $(1/35)^{1/4} \approx 0.4$ and $(1/10)^{1/2} \approx 0.3$.

Melting of a quantum mechanical object at $T = 0$.

Mapping:

$2D$ the quantum problem of interacting particles can be mapped on the classical problem of interacting elastic lines directed along the z-coordinate in $3D$ space. A world line of a two-dimensional particle is isomorphic to the trajectory of the elastic line in three space dimensions.

The Feynman path integral for a fluid of interacting particles in $2D \rightleftarrows$

$\rightleftarrows$ the partition function of the arrays of the directed lines in $3D$

$$\frac{1}{\hbar} \int m \left(\frac{d\mathbf{r}}{dt} \right)^2 dt \rightleftarrows \frac{1}{kT} \int \kappa \left(\frac{d\mathbf{u}}{dz} \right)^2 dz \tag{56}$$

Here the $2D$ vector $\mathbf{u}(\mathbf{z})$ describes a deviation of the elastic line from the position of equilibrium, and κ is the coefficient of elasticity.

$$\frac{1}{\hbar} \int_0^{\beta_{2D}} m d\tau \rightleftarrows \frac{1}{kT_{3D}} \int_0^{L} \kappa dz \tag{57}$$

(Here $\beta_{2D} = 2\pi/T_{2D}$ has nothing in common with T_{3D}. In the mapping $T_{2D} \rightarrow 0$ if L, the length of the $3D$ lines, tends to zero; T_{3D}, which has as a counterpart $\hbar$, remains finite.) Mostly, the trajectories are slightly wiggling lines, but sometimes they entangle each other. Eventually this leads to melting.

The system of lines is more stable against fluctuations than a crystal made of discrete points.

Lindemann criteria for melting of arrays of lines:

$\left\langle \delta r^2 \right\rangle^{1/2} /a$ is about 0.3 rather than 0.15.

B. Negative compressibility (many people were confused).

Perhaps should be said: negative *chemical* compressibility.

$\partial \mu / \partial n$ is negative for not too large values of r_s.

Problem:

$$K^{-1} = \lambda = n^2 \partial \mu / \partial n \tag{58}$$

negative compressibility means an instability.

Condensed matter system as a set of springs with a distributed mass.

Capacitance measurements:

in $GaAs$ heterostructures, $\partial \mu / \partial n$ becomes negative at $n \lesssim 10^{11} cm^{-2}$, i.e., $r_s \gtrsim 2$.

(Unlike the spin susceptibility, the conclusion about negative compressibility, appeared to be not a consequence of inaccuracy of the calculations.)

The resolution of the "paradox":

(i) electric term

$\frac{1}{2} \int \delta n(\mathbf{r}) V_C(\mathbf{r} - \mathbf{r}') \delta n(\mathbf{r}') d\mathbf{r} d\mathbf{r}'$

(ii) "material" or "chemical" term originating from the expansion of the local energy,

$\frac{1}{2} \int \lambda \frac{(\delta n(\mathbf{r}))^2}{n^2} d\mathbf{r} = \frac{1}{2} \int (\delta n(\mathbf{r}))^2 \frac{\partial \mu}{\partial n} d\mathbf{r}$

The actual condition of stability

$$\frac{\partial \mu}{\partial n}(q) + V_C(q) > 0. \tag{59}$$

Why all that is so artificial?

After all, many condensed systems have itinerant electrons.

The condition of stability in the simplest case of a capacitor with the $2D$ gas on one side and the gate on the other:

$$e^2 C_{measured}^{-1} = \left(e \frac{\partial \varphi}{\partial n} + \frac{\partial \mu}{\partial n} \right) > 0, \tag{60}$$

$C_{measured}^{-1}$ is the inverse of the capacitance per square

the two terms on the right hand side describe the response of the electrical and potentials, respectively.

$$e^2 C_{measured}^{-1} = (e^2 C_{geometrical}^{-1} + \frac{\partial \mu}{\partial n}) > 0, \tag{61}$$

valid only for modulation with $q < 1/d$.

Finally

$$\frac{\partial \mu}{\partial n}(q) + \min \left\{ V_C(q), e^2 C_{geometrical}^{-1} \right\} > 0. \tag{62}$$

C.   Physics at short scales

For a distant electrode, a question arises about finite q.

What about the q-dispersion of $\partial \mu / \partial n$?

($\partial n/\partial \mu = \pi(q)$ the polarization operator of electrons)

The most natural behavior for $\partial \mu/\partial n$ in the case of the strong interaction, is that it starts from a negative value, passes through zero, and then continues to increases.

Can the two curves $\frac{\partial \mu}{\partial n}(q)$ and $-V_C(q)$ touch each other?

The compressibility of the Wigner crystal

$$\frac{\partial \mu}{\partial n}(q=0)_{\text{Wigner crystal}} = -2.21 \frac{3\pi r_s}{8m}. \tag{63}$$

In the experiment the compressibility changes its trend at $r_s \gtrsim 4.5$.

comment about the MI transition

For free electrons the compressibility stands constant as far as $q < 2k_F$.

$-V_C(q = 2k_F) = -\pi r_s/\sqrt{2}$

$\partial \mu/\partial n$ as a function of q it starts deeper than $-V_C(q = 2k_F)$.

There is a chance that the two curves indeed intersect at large enough r_s.

The moment of touching of the two curves means that a modulation of density starts to develop.

CDW

SDW

Two scenarios (assuming that the Wigner crystal is an ultimate solution):

(i) the gradual modulation of density eventually develops into the Wigner crystal

(ii) the Wigner crystal intervenes through the first order phase transition.

The Mexican-hat story in the theory of the solidification via CDW, stripes, etc.

Next circle: like Wigner crystal "sits" inside the quantum liquid hidden by fluctuations, it may be that correlations a la CDW or SDW exist much before they become visible as a result of the phase transition.

Possibly for electrons in high Tc-systems.

Screening in Electron Liquids

D. Screening as a condition of equilibrium

Screening, generally, is the result of response of a system of itinerant charges on an external potential $\varphi_{\text{probe}}(\mathbf{r})$.

φ_{probe} induces a redistribution of their density, $\delta n(\mathbf{r})$. Together with the potential φ_{probe} the induced charges create a potential $\varphi_{\text{scr}}(\mathbf{r})$.

$\varphi_{\text{scr}}(\mathbf{r})$ is not an ultimate product of the presence of φ_{probe}. The material part of the liquid (everything that is not related to electrostatic interactions, e.g., kinetic energy of electrons) changes as a result of the redistribution of the density.

This leads to a change in the chemical potential which is equal to

$$\delta\mu(q) = \delta n(q)\frac{\partial\mu}{\partial n}(q), \tag{64}$$

Together the three contributions: (i) φ_{probe}, (ii) potential of induced charges $\equiv (\varphi_{\text{scr}} - \varphi_{\text{probe}})$, plus (iii) $\delta\mu(q)$ should be equal zero.

$$\varphi_{\text{probe}} + (\varphi_{\text{scr}} - \varphi_{\text{probe}}) + \delta n(q)\frac{\partial\mu}{\partial n}(q) = 0. \tag{65}$$

The equality implies that the electrochemical potential in the equilibrium is kept constant over the space.

The two coupled equation should be solved

$$(\varphi_{\text{scr}} - \varphi_{\text{probe}}) = \delta n(q)V_C(q), \tag{66}$$

$$\delta n(q) = \frac{-\varphi_{\text{probe}}(q)}{\frac{\partial\mu}{\partial n}(q) + V_C(q)}. \tag{67}$$

Finally,

$$\varphi_{\text{scr}} = \frac{\varphi_{\text{probe}}\frac{\partial\mu}{\partial n}(q)}{\frac{\partial\mu}{\partial n}(q) + V_C(q)} \equiv \frac{\varphi_{\text{probe}}}{1 + \frac{\partial n}{\partial\mu}(q)V_C(q)}. \tag{68}$$

$\left(\frac{\partial\mu}{\partial n}(q) + V_C(q)\right) > 0$ ensures the stability of the system

A condensed matter system as a set of elastic strings: $\delta n(q)$ has a sign opposite to a probe charge e_0 creating φ_{probe}. The stable system provides a response opposing the perturbation as it should be.

Hohenberg and Kohn "Inhomogeneous Electron Gas" Phys. Rev. 136, B 864 (1964).

"This paper deals with the ground state of an electron gas in an external potential $v(r)$. It is proved that there exists a universal function of density, $F[n(r)]$, independent of $v(r)$, such that the expression $E \equiv \int v(r)n(r) + F[n(r)]$ has as its minimum value the correct ground-state energy associated with $v(r)$. The functional $F[n(r)]$ is then discussed for two situations: (1) $n(r) = n_0 + \widetilde{n}(r)$, $\widetilde{n}/n_0 \ll 1$, ...This approach also shed light on generalized Thomas-Fermi screening methods and their limitations..."

A non-trivial jump: instead of a complicated quantum-mechanical problem, a classic system under the condition that its quantum-mechanically averaged density is $n(\mathbf{r})$.

For a given potential $\varphi_{\text{external}}(\mathbf{r})$, which is not obligatory small, the energy functional

$$E_{\varphi_{\text{external}}}[n(\mathbf{r})] \equiv \int \varphi_{\text{external}}(\mathbf{r})n(\mathbf{r})d\mathbf{r} + F[n(\mathbf{r})], \tag{69}$$

where

$$F[n(\mathbf{r})] = \frac{1}{2}\int \frac{\delta n(\mathbf{r})\delta n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}' + \frac{1}{2}\int \delta n(\mathbf{r})K(\mathbf{r}-\mathbf{r}')\delta n(\mathbf{r}')d\mathbf{r}d\mathbf{r}' + \tag{70}$$

$$\frac{1}{2}\int \delta n(\mathbf{r})\delta n(\mathbf{r}')\delta n(\mathbf{r}'')L(\mathbf{r},\mathbf{r}',\mathbf{r}'')d\mathbf{r}d\mathbf{r}'d\mathbf{r}'' + ... \tag{71}$$

The inverse of the kernel $K(\mathbf{r}-\mathbf{r}')$ is determined by the irreducible (with respect to the Coulomb interaction) density-density correlation function $\langle\delta n(\mathbf{r})\delta n(\mathbf{r}')\rangle$.

In the usual terminology this correlation function is called the polarization operator $\pi(q)$, and as such used instead of $\frac{\partial n}{\partial \mu}(q)$.

From the condition for equilibrium one has

$$\varphi_{\text{external}}(\mathbf{r}) + \int \frac{\delta n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \delta F[n]/\delta n(\mathbf{r}) = \mu_{\text{el-chem}}. \tag{72}$$

The first two terms constitutes the electric potential of charges, the last one represents the chemical potential.

$\mu_{\text{el-chem}}$ is the electro-chemical potential, which is maintained to be spatially constant.

To proceed further one need to know the "material" part of $F[n]$. The simplest approximation: $\delta F[n]/\delta n(\mathbf{r}) = E_F^{\text{free}}[n(\mathbf{r})]$. Then, from the condition for equilibrium one has

$$\varphi_{\text{external}}(\mathbf{r}) + \int \frac{\delta n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + E_F^{\text{free}}[n(\mathbf{r})] = \mu_{\text{el−chem}}. \tag{73}$$

Finally, one rewrites all that in the form of two self-consistent equations:

$$n(\mathbf{r}) = n^{\text{free}}[\mu_{\text{el−chem}} - \varphi_{\text{external}}(\mathbf{r}) - \varphi_{\text{induced}}(\mathbf{r})], \tag{74}$$

$$\varphi_{\text{induced}}(\mathbf{r}) = \int \frac{\delta n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'. \tag{75}$$

Historically, it the set of two equations was written by Thomas and Fermi using locality and the argumentation which is called self-consistency.

"But where is this self-consistency?"

The same quantity $\delta n(\mathbf{r})$ creates $\varphi_{\text{induced}}(\mathbf{r})$ and maintains the equilibrium.

E. Screening as an infinitely repeating process of polarization

$$\varphi_{\text{scr}}(q) = \frac{\varphi_{\text{probe}}(q)}{1 + V_C(q)\pi(q)}. \tag{76}$$

Instead of $\frac{\partial n}{\partial \mu}(q)$ people use the term polarization operator $\pi(q)$.

Why?

If formally expand $\varphi(q)$ with respect to $V_C(q)$, one gets a geometrical series:

$$\varphi(q)_{\text{scr}} = \varphi_{\text{probe}}(q) - \varphi_{\text{probe}}(q)\pi(q)V_C(q) + \varphi_{\text{probe}}(q)\pi(q)V_C(q)\frac{\partial n}{\partial \mu}(q)V_C(q)...$$

It turns out that in order to describe screening it is not possible to be limited to any finite order in e^2.

"Why did not we notice this infinite series in the self-consistent derivation of the effect of screening".

A remark about self-consistency.

Generating of the repeating process in the case of screening.

Reminding: by varying $\mu(r)$, one introduces in the Hamiltonian the term $\delta\mu(\mathbf{r})n(\mathbf{r})$. Therefore, finding of $\frac{\partial n}{\partial \mu}(q) \equiv \pi(q)$ reduces to the calculation of the density-density correlation function (irreducible with respect to a single Coulomb interaction line).

For free electrons $\frac{\partial n}{\partial \mu}(q=0) = 2\nu$, where ν is the density of states per one spin species.

The need in summation of the infinite series versus the perturbation with respect to the small parameter $e^2/\hbar v_F$.

Does it actually work?

All virtual states with more than one electron-hole pair in the process of polarization can be treated perturbatively.

For a point-like probe charge e_0

$$\varphi_{\text{scr}}^{3D}(q) = 4\pi e_0/(q^2 + 4\pi e^2 \frac{\partial n}{\partial \mu}(q)). \tag{77}$$

It is regular at $q \to 0$

$$\varphi_{\text{scr}}(q) = 4\pi e_0/(q^2 + \varkappa_{\text{scr}}^2); \qquad \varkappa_{\text{scr}} = \left(4\pi e^2 \frac{\partial n}{\partial \mu}(q \to 0)\right)^{1/2}. \tag{78}$$

!!!

$$!!! \qquad e^2/\hbar v_F \ll 1 \qquad \rightleftarrows \qquad \varkappa_{\text{scr}} \varkappa_{\text{scr}} \ll k_F \qquad !!! \tag{79}$$

The Fourier transform of $\varphi_{\text{scr}}(q)$. For $\pi(q)$ its value at $q \approx 0$. Then, pole at an imaginary $q_{\text{pole}} = \pm i \varkappa_{\text{scr}}$

$$q_{\text{pole}} \implies \varphi_{\text{scr}}(r) = \frac{e_0}{r} \exp(-\varkappa_{\text{scr}} r), \tag{80}$$

$\varkappa_{\text{scr}}$ acquires the meaning the inverse radius of screening

$$r_{\text{scr}} = \left(4\pi e^2 \frac{\partial n}{\partial \mu}(q \to 0)\right)^{-1/2}; \qquad r_{\text{scr}} = \varkappa_{\text{scr}}^{-1}. \tag{81}$$

Most important:

the inequality $e^2/\hbar v_F \ll 1$ implies that the screening cloud is very extended, i.e., its radius exceeds much the inter-particle distance. Under the condition $r_{\text{scr}} = \left(\frac{1}{4\pi e^2} \frac{\partial \mu}{\partial n}(q \to 0)\right)^{1/2} \gg r_0$, the local Thomas-Fermi approximation has firm grounds.

Role of the Fermi statistic. A need in the energy scale.

The Debye-Huckel radius of screening is equal to $(\frac{T}{4\pi e^2 n})^{1/2}$.

Fermi statistic provides us with an energy scale (E_F instead of T).

Exponential screening with a finite screening length is not the whole and not true story. Friedel oscillations.

The end of the firm territory $e^2/\hbar v_F \ll 1$.

F.   Screening when the compressibility is negative

In the case when $\frac{\partial \mu}{\partial n}(q \to 0) < 0$ the blind application of the standard formula $\varphi_{\text{total}}(r) = \frac{e_0}{r}\exp(-r/r_{scr})$ leads to a pathological result

$$\varphi_{\text{total}}(r) = \frac{e_0}{r}\cos \varkappa r \qquad \Longrightarrow \text{absurd} \tag{82}$$

"why not?   It is an overreacting system.

Why not to imagine this formula as a result of a poorly convergent procedure."

An erroneous idea. What is the *trend?*

How can it be that it disappears at all?

All Fourier components of the induced charge density provides a response with a sign opposing the perturbation:

$$\delta n(q) = \frac{-\varphi_{\text{probe}}(q)}{\frac{\partial \mu}{\partial n}(q) + V_C(q)}, \tag{83}$$

No accumulation of a charge with a wrong sign. The screening cloud exactly compensates (i.e., equal and opposite) the one creating the external potential.

The standard looking result

$$\varphi_{\text{scr}} = \frac{\varphi_{\text{probe}}\frac{\partial \mu}{\partial n}(q)}{\frac{\partial \mu}{\partial n}(q) + V_C(q)} \equiv \frac{\varphi_{\text{probe}}}{1 + \frac{\partial n}{\partial \mu}(q)V_C(q)}. \tag{84}$$

!!!

when the compressibility is negative: potentials φ_{scr} and $\varphi_{\text{external}}$ have opposite signs.

!!!

What is my purpose, now.

I try to show that the description of screening how it was done in the past by Debye and Huckel is not the only one.

The point is how to solve the set of two equation $\varphi_{\text{probe}}(\mathbf{r}) + \varphi_{\text{induced}}(\mathbf{r}) = \varphi_{\text{scr}}(\mathbf{r})$ and $\varphi_{\text{scr}}(\mathbf{r}) + \varphi_{\text{chem}}(\mathbf{r}) = 0$ perturbatively.

In the standard route, one first equalizes $\varphi_{\text{probe}}(\mathbf{r})$ with $\varphi_{\text{scr}}(\mathbf{r}) = -\varphi_{\text{chem}}(\mathbf{r})$ and treat $\varphi_{\text{induced}}(\mathbf{r})$ as a correction.

Instead of the Debye-Huckel route, one can first equilibrate $\varphi_{\text{probe}}(q)$ with $-\varphi_{\text{induced}}(q) = -\delta n(q) V_C(q)$.

We first totally compensate $\varphi_{\text{probe}}(q)$ as if the electron liquid is a classical gas at $T = 0$ and $r_{\text{scr}} = 0$.

$\varphi_{\text{chem}}(\mathbf{r})$ as a correction. The infinite series is looking as

$$\varphi(q)_{\text{scr}} = 0 + \varphi_{\text{probe}}(q)\frac{\partial \mu}{\partial n}(q)/V_C(q) - \varphi_{\text{probe}}(r)\left(\frac{\partial \mu}{\partial n}(q)/V_C(q)\right)^2 + ... =$$
$$\varphi_{\text{probe}}(r)\frac{\partial \mu}{\partial n}(q)/[V_C(q) + \frac{\partial \mu}{\partial n}(q)]$$

The obtained expansion is less defected at small q, especially for $\partial \mu/\partial n < 0$ (unless the system is unstable) and has a clear physical meaning.

Let us discuss what we will get for the total potential if we take for $\frac{\partial \mu}{\partial n}(q)$ as a smooth analytic function of q.

From the stability condition that there cannot be real q_0 such that $[V_C(q_0) + \frac{\partial \mu}{\partial n}(q_0)] = 0$.

[!!!This is in a strong contrast with what one got assuming naively that $\frac{\partial \mu}{\partial n}(q) = const < 0$ and that lead to the pathological result $V_C^{\text{screen}}(r) = \frac{e}{r}\cos(r/r_{scr})$.!!!]

A pole is located in the complex plane somewhere in a general point not related to the value of $\pi(q = 0)$.

When converted into the coordinate space (under assumption that $\frac{\partial n}{\partial \mu}(q)$ is analytic), $\varphi(q)_{\text{scr}}$ produces an exponential decaying potential. Indeed, with oscillations, but still exponentially decaying.

Conclusion: the negative (chemical) compressibility does not create big troubles in a system with itinerant charges till the latter is far from the boundary of stability $[V_C(q) + \frac{\partial \mu}{\partial n}(q)] > 0$.

G.   Other oscillations and screening in $2D$

In order to find the far-tail of the screening cloud $\delta n(\mathbf{r})$, one has to calculate the Fourier transform of $\delta n(q) = -\varphi_{\text{probe}}(q)/\left(\frac{\partial \mu}{\partial n}(q) + V_C(q)\right).$

The sharp Fermi surface leads to a non-analytical behavior in $\pi(q)$ at $q = 2k_F$.

A general phenomenon related to a jump in the occupation numbers $n(p)$.

The non-analyticity sitting in the polarization operator shows up, and it provides a contribution which oscillates with the period $(2k_F)^{-1}$ and decays as $1/r^D$.

The Friedel oscillations are detected in the NMR measurements. One should not be confused:

Relation between $S(q)$: the polarization operator $\pi(q)$ is calculated in the limit $\omega = 0$. This correlation function is more singular.

The non-analyticity in $\pi(q)$ in different dimensions:

in $3D$ a logarithmic singularity in the derivative at $q = 2k_F$;

in $2D$ the polarization operator has a cusp at $2k_F$;

in $1D$ it even diverges logarithmically.

The screening in $2D$.

Only electrons are confined in the layer.

For a probe charge e_0, its screened potential in $2D$ is equal to

$$\varphi_{\text{scr}}(q) = 2\pi e_0/(|q| + 2\pi e^2 \frac{\partial n}{\partial \mu}(q)). \tag{85}$$

Like in $3D$, it can be written as

$$\varphi_{\text{scr}}(q) = 2\pi e_0/(|q| + \varkappa_{\text{scr}}); \qquad \varkappa_{\text{scr}} = 2\pi e^2 \frac{\partial n}{\partial \mu}(q \to 0). \tag{86}$$

Also like in $3D$, the condition $e^2/\hbar v_F \ll 1$ implies that $\varkappa_{\text{scr}} \ll k_F$.

On that point the similarity ends.

The Fourier transform leads to special functions. (It was done by F.Stern and can be found in the encyclopedian review published in Rev. Mod. Physics.) Obviously, there will be oscillations with the period $\varkappa_{\text{scr}}$.

An answer on a crude-picture question: "what is in place of the exponentially decaying potential?"

The cloud is located within the plane. Therefore, it cannot screen all the multiplets of the probe potential. Part of the electric field flows away through the third direction.

As a result the screened potential decays as $1/r^3$.

Why do we care about the convental screening with its exponential decay in $3D$ or $1/r^3$ in $3D$ theses tails are much weaker than those produced by the Friedel oscillations?

The $2k_F$ non-analyticity is a rather subtle thing.

On the contrary, the conventional screening is a very robust mechanism, and it guarantees supplying of charge cloud to oppose the external perturbation.

H. What other charges do?

Other charges can shift from the position of equilibrium, and in this way participate in screening.

The simplified functional $E_{\varphi_{\text{external}}}$ should be extended by the new terms:

$$E_{\varphi_{\text{external}}}[n(\mathbf{r})] \equiv \int \varphi_{\text{external}}(\mathbf{r})n(\mathbf{r})d\mathbf{r} - \int \varphi_{\text{external}}(\mathbf{r})N(\mathbf{r}) + F[n(\mathbf{r}); N(\mathbf{r}')], \tag{87}$$

where $F[n(\mathbf{r}); N(\mathbf{r}')] = F[n(\mathbf{r})] + F[N(\mathbf{r}')] + F_{\text{mixed}}[n(\mathbf{r}); N(\mathbf{r}')]$.

$$F[N(\mathbf{r}')] + F_{\text{mixed}}[n(\mathbf{r}); N(\mathbf{r}')] = \frac{1}{2}\int \frac{\delta N(\mathbf{r})\delta N(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}d\mathbf{r}d\mathbf{r}' + \frac{1}{2}\int \delta N(\mathbf{r})K_+(\mathbf{r} - \mathbf{r}')\delta N(\mathbf{r}')d\mathbf{r}d\mathbf{r}' \tag{88}$$

$$- \int \frac{\delta n(\mathbf{r})\delta N(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}d\mathbf{r}d\mathbf{r}' + ... \tag{89}$$

The term K_+ includes chemistry like the covalent bonds.

One has to find the condition for equilibrium by variation with respect to $\delta n(\mathbf{r})$ and $\delta N(\mathbf{r}')$. Going directly to the Fourier transform one gets a pair of equations.

$$\varphi_{\text{external}}(q) + \delta n(q)V_C(q) + \delta n(q)K_{el}(q) - \delta N(q)V_C(q) = 0 \tag{90}$$
$$-\varphi_{\text{external}}(q) + \delta N(q)V_C(q) - \delta n(q)V_C(q) + K_+\delta N(q) = 0 \tag{91}$$

Substraction yields

$$\varphi_{\text{external}}(q) + [\delta n(q) - \delta N(q)]V_C(q) + \frac{1}{2}[\delta n(q)K_{el}(q) - K_+\delta N(q)] = 0 \tag{92}$$

Note that $[\delta n(q) - \delta N(q)]$ is the induced charge density of the two species, and $[\delta n(q) - \delta N(q)]V_C(q) = \varphi_{\text{induced}}(q)$.

Finally,

$$\varphi_{\text{scr}}(q) = \varphi_{\text{external}}(q)\frac{(1/K_{el} + 1/K_+)^{-1}}{V_C + (1/K_{el} + 1/K_+)^{-1}}. \tag{93}$$

The compressibility of the electrons and charged ions/dopants comes symmetrically in the screened potential.

In the case of ions there are absolutely no reasons to neglect the contribution of $1/K_+$ in the total compressibility. This term also participates in the stability of the system.

This is not the case for the semiconductors. The energy scales of the itinerant of electrons (typically $\sim 100K$) are much smaller than the energy of the chemical bonds controlling the rigidity of the host lattice keeping the dopants (typically $\sim 1eV$). Therefore, $K_{el} \ll K_+$ and the screening is determined by the itinerant electrons only.

I.   Remarks about non-linear screening

asymmetry of $+e$ and $-e$ at large r_s.

fluctuations the bottom of the band created by remote donors separated by the spacer s :

$$1/\sqrt{|r^2| + s^2} \rightleftarrows \frac{2\pi}{|q|} \exp(-|q|\,s)$$

Screening of this fluctuations.

J.   Last remark:

When a given bias voltage is applied, it is the difference in the electrochemical potential. The charges are forced to arrange themselves in such a way that they produce the difference in the electrochemical potential equal to a given voltage.

Tonnes of wrong papers!

IV.   LITERATURE

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