Metal–Insulator Transition in quasi 2D

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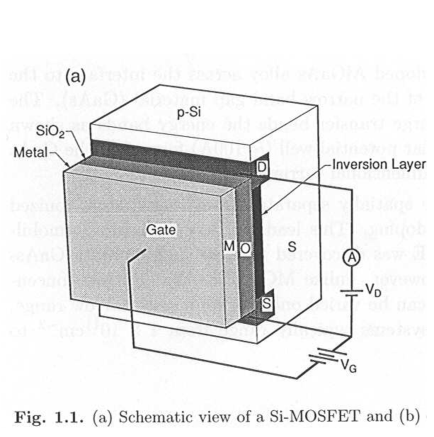
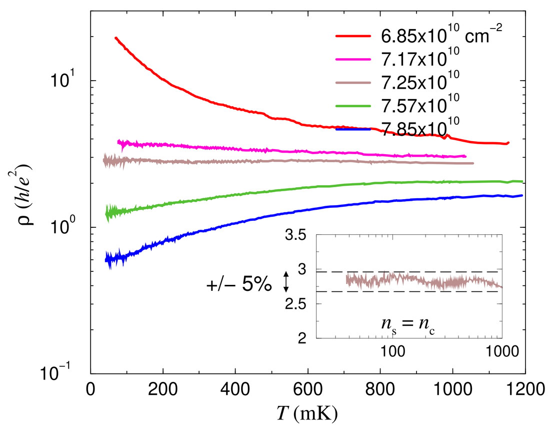
MAX-PLANCK-GESELLSCHAFT

Metal-Insulator transition



From [1]



Resistivity vs. temperature for different electron densities in Si MOSFET [2]

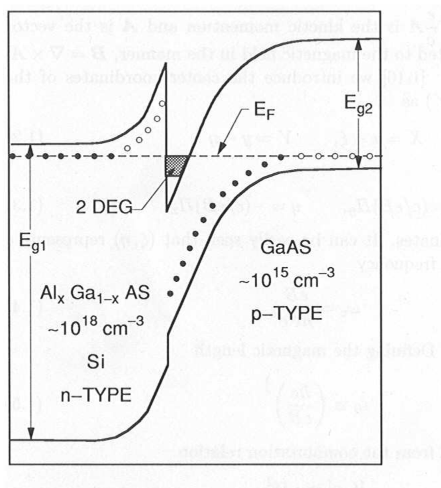


Fig. 1.2. Energy diagram at a GaAs-heterostructure interface

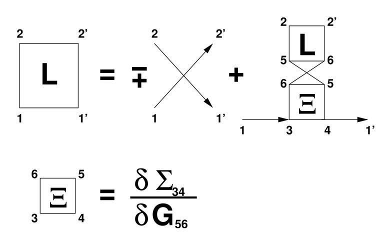
Model

- Quasi-2D electron gas (cylindrical Fermi surface)
- Localization (Insulator) – Delocalization (Metal) transition as Mott transition
- Electron interacts with charged and neutral impurities

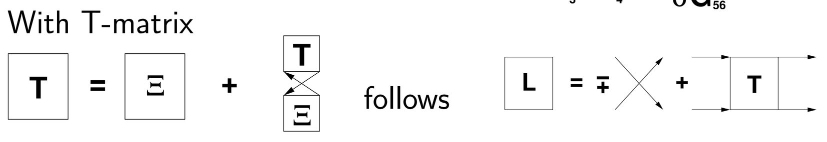
General Response function

Variation with respect to the external potential, density fluctuation

$$L_{121'2'} = G_{121'2'} - G_{11'}G_{22'} = \mp\frac{\delta G_{11'}}{\delta U_{2'2}} =$$

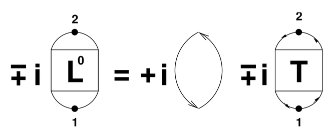


With T-matrix



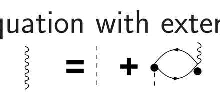
Response function

$$\chi_{12} = \frac{\delta n_1}{\delta U_{22}} = \mp i L_{121+2} =$$

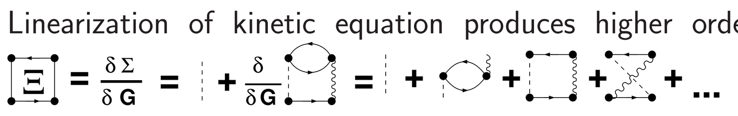


Advantage of kinetic theory - strategy:

- Kinetic equation with external field and many-body approximation

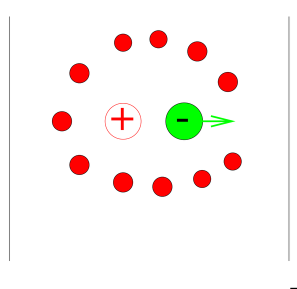
  GW: 

- Linearization of kinetic equation produces higher order correlations

- Direct access to conductivity by balance equation

Debye-Onsager-Relaxation-Effect in plasmas



Screening cloud retarded- dipole force

Debye '23 [3] $E\,(1-\frac{\kappa e^2}{6\epsilon_0 T})$
Onsager '27 [4] $E\,(1-\frac{\kappa e^2}{3(2+\sqrt{2})\epsilon_0 T})$

Treatment within quantum kinetic theory [5–8]

$$\frac{\partial}{\partial t}f - e\,\mathbf{E}\frac{\partial}{\partial \mathbf{k}}f = I[f(\mathbf{k}-\mathbf{p}),\mathbf{E}]$$

Balance of current $\mathbf{J} = n\frac{e}{m}\mathbf{p}$

$$\frac{\partial}{\partial t}\mathbf{p} + en\mathbf{E} = R(E,t)en\,\mathbf{J} + en\frac{\delta E(E,t)}{E}\mathbf{E}$$

Conductivity beyond linear response [8] $\sigma(E) = \frac{1-\frac{\delta E(E)}{E}}{R(E)}$

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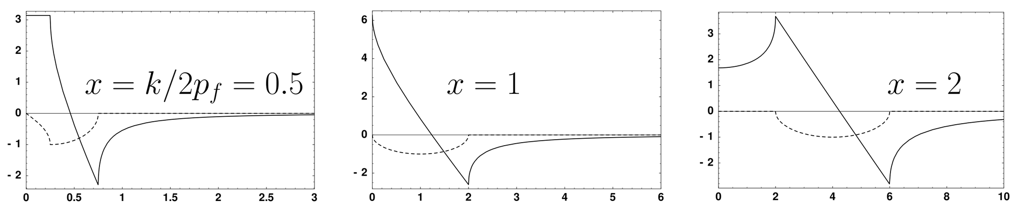
Selfenergy

Potential $V(q) = 2\pi e_a e_b/q$ for charged impurities, $\mathcal{E} = 1 - V\Pi$

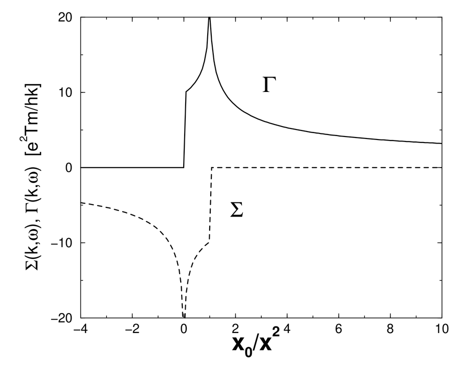


Classical fluctuations $\Pi^{\gtrless}(\omega,k) = \pm 2g(\pm\omega)\mathrm{Im}\Pi(\omega,k) \approx \frac{2T}{\omega}\mathrm{Im}\Pi(\omega,k)$

$$\Sigma^{\gtrless}(\omega,k) \;=\; -2\pi T\int\frac{dq}{(2\pi)^2}V_{aa}(q)\mathrm{Re}\left(1-\frac{1}{\mathcal{E}(q,0)}\right)f^{\gtrless}_{k-q}\delta(\epsilon_{k-q}-\omega)$$

Result

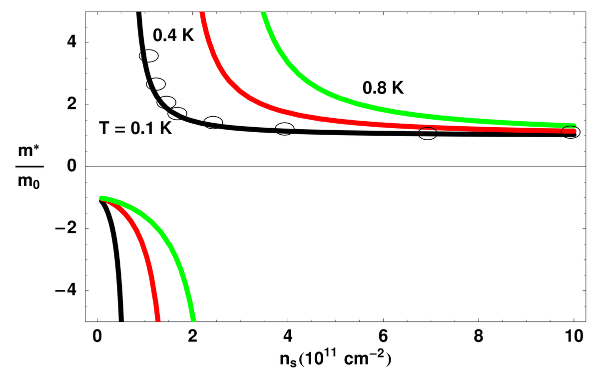
$$\Sigma(\omega,k) = \frac{2\pi e_a^2 T_b m_a}{\hbar p_f(x+\sqrt{x_0})}\mathcal{K}\left[\left(\frac{\sqrt{x_0}-x}{\sqrt{x_0}+x}\right)^2\right] \to 2\pi^2 T\kappa_a \quad \text{for} \quad \omega = \epsilon_f$$



Real and imaginary part of first temperature correction of selfenergy versus scaled frequency $x_0/x^2 = 2m\hbar\omega/k^2$, $\kappa_a = \frac{\hbar\kappa}{2p_f}$

Effective mass

$$\frac{m}{m^*} = \frac{\frac{1}{m}+\frac{1}{k}\frac{\partial\Sigma}{\partial k}}{1-\frac{\partial\Sigma}{\partial\hbar\omega}} = \frac{1-\frac{1}{4\epsilon_{fa}}\Sigma(p_f,\epsilon_f)}{1+\frac{1}{4\epsilon_f}\Sigma(p_f,\epsilon_f)} \approx 1-\frac{1}{2\epsilon_f}\Sigma(p_f,\epsilon_f)$$



The effective mass for temperatures $0.1, 0.4, 0.8$K from left to right [9] . The open circles are experimental values of [10].

$\sigma = \frac{e^2}{m}n\tau$: Mott-Hubbard transition, $m \to \infty$, rather than Anderson, $n\tau \to 0$,

Conductivity and Relaxation Effect

$$\sigma(E) = \frac{n_a e_a^2}{m_a}\tau\left(1-\frac{\delta E}{E}\right)$$

Statical Screening - Neutral impurities

the low density expansion $a_0 = -2m_a g_{ai} r_0^2/\hbar^2$

$$\tau_i^{-1}\frac{m_a}{n_a e_a^2}\frac{e_a^2}{h} = \frac{2^{3/2}s_i n_i}{s_a n_a}\left(\frac{-a_0}{2r_0}\right)^2\left\{1-\frac{\pi}{2\kappa_i}-\frac{\pi^2}{24}\frac{T^2}{e_f^2}\frac{\pi^3}{16\kappa_i}+o(\kappa_i^{-4})\right\}$$

$$\frac{\delta E}{\delta E} = \frac{n_i}{n_a}\left(\frac{-a_0}{2r_0}\right)^2\left\{1+\frac{4-3\ln 2\kappa_i}{\kappa_i^2}+o(\kappa_i^{-4})\right\}$$

Dynamical Screening - charged impurities

$$\tau_{ab}^{-1}\frac{m_a}{n_a e_a^2}\frac{e_a^2}{h} = \frac{8s_b}{s_a^3}\left(\frac{T_a}{\epsilon_f}+\frac{T_b}{\epsilon_f}\right)\kappa_a\left(1-\frac{\pi}{4\kappa_a}+\frac{2}{3\kappa_a^2}+o(\kappa_a^{-3})\right)$$

$$\frac{\delta E}{E} = -\frac{2s_b}{s_a^2}\left(\frac{T_a}{\epsilon_f}+\frac{T_b}{\epsilon_f}\right)\left(-1+(\ln(2\kappa_a)-1)\frac{1}{\kappa_a^2}+o(\kappa_a^{-4})\right)$$

Since $\kappa_a = \frac{\hbar\kappa}{2p_f} = \sqrt{\frac{\hbar}{\tau_0\epsilon_f}}$ $\quad \frac{1}{\tau_0} = \frac{me_a^2e_b^2s^2}{8\hbar^3}$
we have $1-\frac{\delta E}{E} = 1-\frac{T}{\epsilon_f}\left(1+\frac{\tau_0\epsilon_f}{2\hbar}\ln\left(\frac{\tau_0\epsilon_f}{4\hbar}\right)\right)$

Comparison with experiment: Trapping

Two unknown fit parameter: energy level $E_b = E_c - E_D$ of impurities determining the ratio of impurity density to electron densities

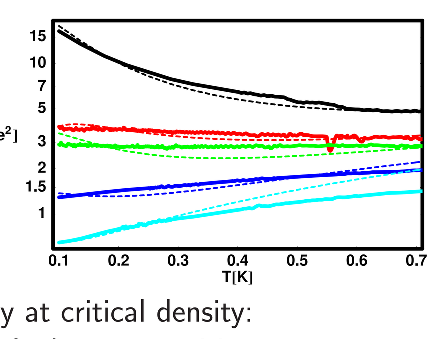
$$\frac{n_i}{n_a} = n_a\left(\frac{2\pi\hbar^2}{m_a T}\right)\mathrm{e}^{\beta E_b}$$

and ratio of scattering length to range of neutral impurities $\zeta = \left(\frac{a_0}{r_0}\right)^2\epsilon_f$ $[s_b = 1, T_b = 0]$

$$\frac{\sigma}{\sigma_0} \;=\; 1-\frac{\zeta}{2T}\mathrm{e}^{E_b/T}-\frac{T}{2\epsilon_f}+\frac{T}{2\epsilon_f\kappa_a^2}\ln\frac{2\kappa_a}{e}$$

$$\sigma_0 \;=\; \frac{e^2}{h}\left(\frac{\zeta}{\sqrt{2}T}\mathrm{e}^{E_b/T}+\frac{T}{\epsilon_f}\left(\kappa_a-\frac{\pi}{4}\right)\right)$$

Experiment (solid lines) [2].
From top to bottom $n_a = 6.85, 7.17, 7.25, 7.57, 7.85\,10^{10}$cm^{-2}.



Sharp drop of effective binding energy at critical density:
Mott-Hubbard transition rather than Anderson transition

Mechanism for trapping ?

Trapping by charged donors [9, 11] or Three particle clustering [12]

Molecular dynamics

- classical molecular dynamics
- quasi 2D electron system with impurities
- use effective quantum potential such that correlation energy is equivalent to the true quantum one in leading order [14]

$$V^{eff}(\vec{r}) \;=\; c\int dx\rho(x)V(x)V(x+r) \qquad \rho(r) = \frac{s}{n}\int\frac{dp}{(2\pi\hbar)^3}e^{\frac{i}{\hbar}pr}f_{\mathrm{FD}}(p)$$

High - temperature limit [13]

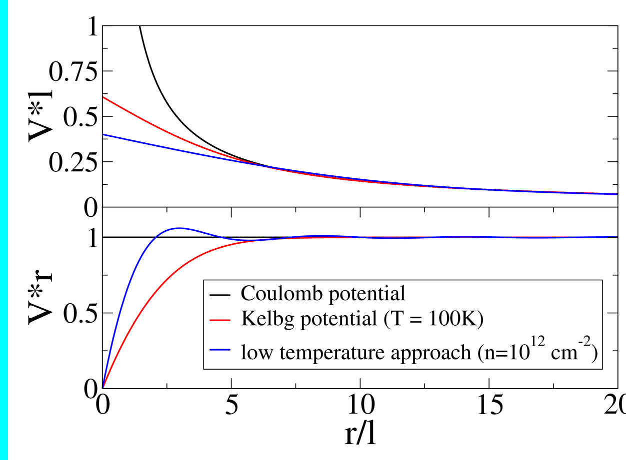
$$\frac{1}{r}\left(1-e^{-(r/l)^2}+\sqrt{\pi}\frac{r}{l}\mathrm{erfc}\left(\frac{r}{l}\right)\right)$$

with $l^2 = 2\hbar^2/mT$

Low - temperature limit [14]

$$\frac{1}{4r}\left(4+\frac{\pi r}{l}-2\cos\left(\frac{r}{l}\right)-\frac{2l\sin\left(\frac{r}{l}\right)}{r}-\frac{2rSn\left(\frac{r}{l}\right)}{l}\right)$$

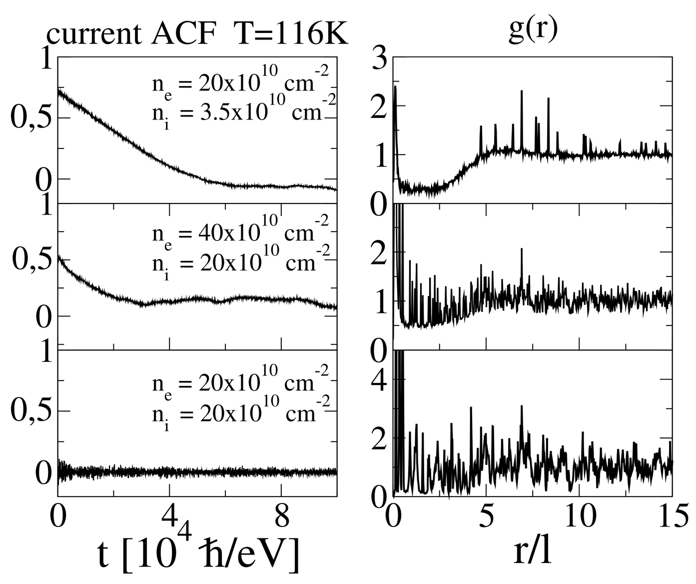
with $l = \frac{\hbar}{p_f}$



no Coulomb divergence by quantum effects at small distances

- conductivity by Kubo formula $\sigma = \frac{ne^2}{kT}\int_0^\infty dt\,\langle j(0)j(t)\rangle_{eq}$
- numerical demanding: high number of verlet steps (at least 10^10) for a converging ACF with a long time decay
- due to pathological dispersion $\omega_p^2 = \frac{4\pi e^2 n}{m}q$

Preliminary results

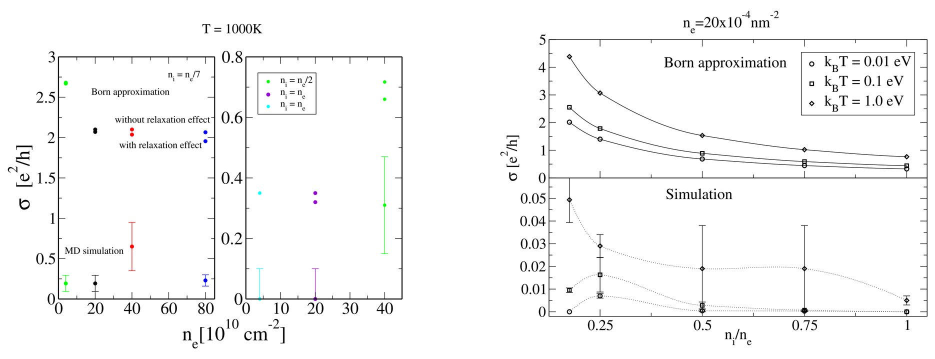


metallic n_e/n_i=1/7

transition n_e/n_i=1/2

insulating n_e/n_i=1

Comparison with Born approximation



- Born approximation yields too high conductivity
- Metal-insulating transition $n_i \approx 0.5 ... 0.7 n_e$

Summary

- GW approximation in kinetic equation leads to higher order diagrams for conductivity by linearization to external field
- Quantum corrections to conductivity by field dependence of collision integral
- Dynamical screening leads to linear temperature dependence, statical screening/neutral scattering leads to Fermi-liquid
- Effective mass described by scattering with charged impurities
- Experimental conductivity and metal-insulator transition as Mott-Hubbard transition
- Mechanism of trapping due to three-particle clustering (magnetic field) or impurity trapping ?
- Observe metal-insulator transition numerically for impurity trapping, but not at half filling

paper available at http://www.mpipks-dresden.mpg.de/~morawetz