Introduction

Thomas-Fermi-Maxwell model

Kohn-Sham model and scalings

Homogenized system - high frequency regime

Homogenized systems - low frequency regime

Dynamics of interacting electrons

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Workshop in CSCAMM, Maryland

Outline

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1. Introduction to the governing equations
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Many-body Schrödinger equation

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In the Born-Oppenheimer approximation,

$$\begin{aligned} i\hbar\frac{\partial\Psi}{\partial t} &= H\Psi = \left(-\frac{\hbar^2}{2m_e}\Delta + V\right)\Psi, \\ V &= V_{ne} + V_{ee} + W. \end{aligned}$$

V_{ne} – the electron-nucleus attraction energy
V_{ee} – the electron-electron repulsion energy
W – the external potential

N electrons $\Longrightarrow$ dimensionality of equation $3N + 1$

Conclusion:

nice equation but mission impossible to be directly solved

Hartree-Fock and TDDFT theory

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Hartree-Fock theory: Ψ has the form of determinant $\{\psi_k\}_{k=1}^N$ – Slater determinant

$$i\hbar\frac{\partial\psi_k}{\partial t} = -\frac{\hbar^2}{2m_e}\Delta\psi_k + V\psi_k,$$
$$V = V_H + V_F + W.$$

V_H - Hartree (Coulomb) potential
V_F - Fock (exchange) operator

TDDFT theory (Runge-Gross theorem, 1984): a unique map between the time-dependent external potential and time-dependent density.

$V = V_{eff}(\rho), \rho = \sum_k |\psi_k|^2 \Longrightarrow$ Thomas-Fermi system (orbital-free) and Kohn-Sham system (orbital-dependent).

Motivations

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- Understand the electron interactions under the picture of Hartree-Fock or TDDFT;
- Derive effective equations in the background of crystals;
- Aim at possible applications in nano-optics and semiconductors.

colors by gold colloids

small spider on small semiconductor

Derivation of the Thomas-Fermi-Maxwell model

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Begin from the quantum many-body action

$$\mathcal{A} = \int < \Psi | i\partial_t - H | \Psi > \, \mathrm{d}t.$$

Take Ψ as the Slater determinant $\{\psi_k\}_{k=1}^N$ and assume $\psi_k = a_k \exp(iS)$ – same phase function,

$$\mathcal{A} = \int \rho \left(-\partial_t S - \frac{1}{2}(A - \nabla S)^2 \right) - < \Psi | H_0 | \Psi > \, \mathrm{d}t,$$

where $\rho = \sum_k |a_k|^2$ we have also considered the magnetic vector potential A in the Hamiltonian

$$H = \frac{1}{2}(i\nabla + A)^2 + V, \qquad H_0 = -\frac{1}{2}\Delta + V.$$

Euler-Lagrange equations

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The Thomas-Fermi approximation of kinetic energy yields,

$$\mathcal{A} = \int \rho \left(-\partial_t S - \frac{1}{2}(A - \nabla S)^2 \right) - C_{TF}\rho^{5/3} - \rho V_c - \epsilon_{xc}(\rho)\,\mathrm{d}t.$$

The Euler-Lagrange equations read as

$$\begin{aligned} &\partial_t \rho + \nabla \cdot (\rho(\nabla S - A)) = 0, \\ &\partial_t S + \frac{1}{2}(\nabla S - A)^2 + \frac{\delta E_{TF}}{\delta \rho} = 0, \\ &E_{TF} = C_{TF} \int \rho^{5/3} + \int \rho V_c + \int \epsilon_{xc}(\rho), \end{aligned}$$

coupled with the Maxwell system

$$\begin{aligned} &\partial_t^2 A - \Delta A + \nabla(\partial_t V_c) = J = \rho(\nabla S - A), \\ &-\Delta V_c = \rho - m, \quad m - \text{nuclei charge}. \end{aligned}$$

Linearized half space problem

(Ritchie, 1973, dispersion of surface plasmon)

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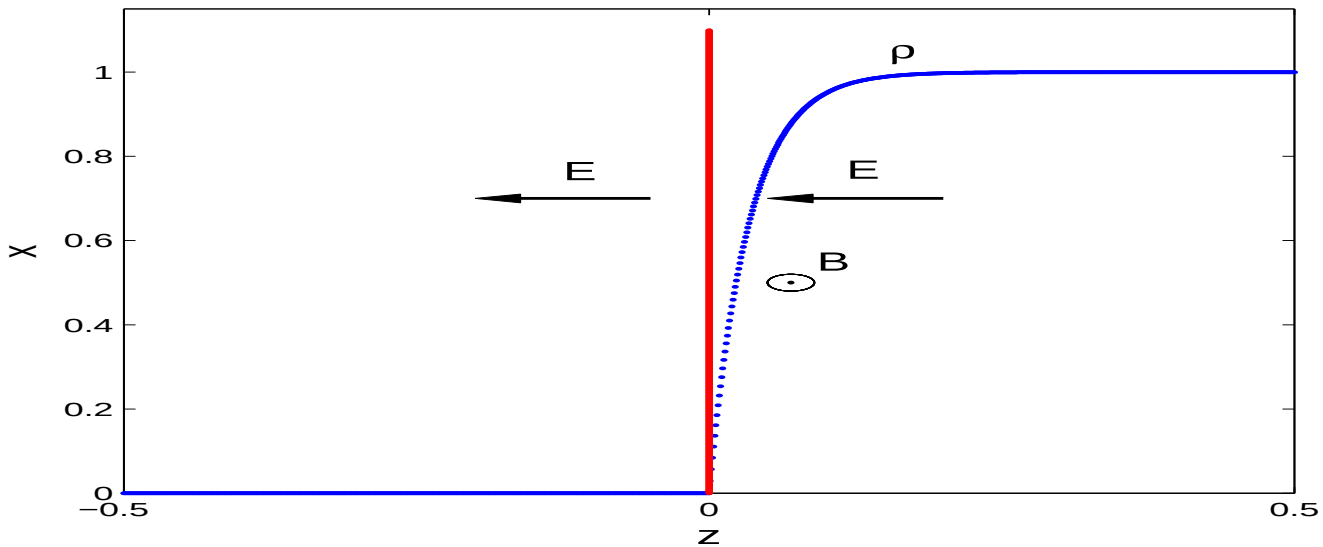
G.S. $\rho_0(x,z) = 1_{z>0}, \quad A = 0, \quad V_c = 0, \quad \nabla S = 0,$

Pert. $E = -\nabla \widetilde{V_c} - \dfrac{\partial \widetilde{A}}{\partial t}, \quad B = \nabla \times \widetilde{A},$

$E = \big(E_1(z), 0, E_3(z)\big) e^{i(kx-\omega t)}, \quad B = \big(0, B_2(z), 0\big) e^{i(kx-\omega t)}.$

Interface condition: E, B are continuous.



Dispersion relation $\omega \sim ? k$

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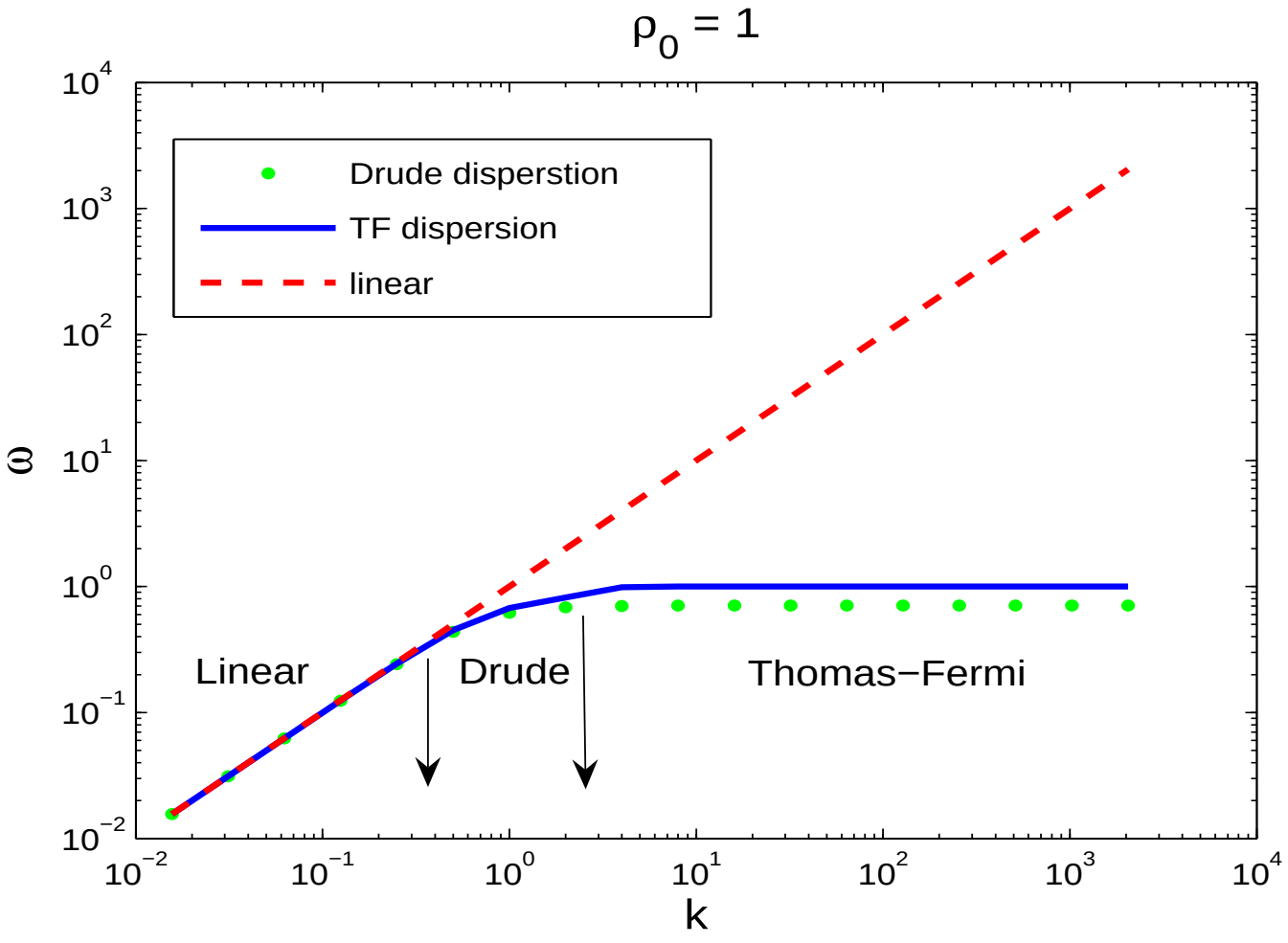

In Drude model electron has classical dynamics

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{p}{\tau} - E, \quad J = \rho_0 p.$$

Discussions on Thomas-Fermi-Maxwell model

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- Both Drude and Thomas-Fermi models lie in the linear regime when the wave number k is small (long waves).
- Out of the linear response regime, Drude model only performs well for a certain range of wave number; as $k \to \infty$ (short waves), one needs to capture the many body effects, for example, by Thomas-Fermi model.
- The nonlinear Thomas-Fermi-Maxwell model could be used to study the optical response of surface plasmon polaritons. (W. Cai and his collaborators)

Kohn-Sham model

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$$i\frac{\partial \psi_j}{\partial t} = -\frac{1}{2}\Delta\psi_j + V_{eff}\psi_j,$$
$$V_{eff} = V_c + W + V_{xc}(\rho),$$
$$-\Delta V_c = \rho - m, \quad \rho = \sum_j |\psi_j|^2 \text{ (spin degeneracy omitted).}$$

ψ_j - the wave function for the j-th independent electron;

V_{eff} - the effective potential; W - the external potential;

V_{xc} - the exchange-correlation potential (with adiabatic local density approximation).

N electrons $\Longrightarrow$ N one body Schrödinger equation.

Goal:

Effective equations modeling electron dynamics in crystals under macroscopic perturbations.

Nondimensionalization - rescalings

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We rescale the system according to the time and length scales of the external potential W.

The length scale $L \gg 1$, and we denote $\varepsilon = 1/L$;

The time scale T distinguishes two regimes

- High frequency: $T = O(1)$.
- Low frequency: $T = O(1/\varepsilon)$;

The rescaled Schrödinger equations are given by

$$i\partial_t \psi_j^\varepsilon = -\tfrac{1}{2}\varepsilon^2 \Delta \psi_j^\varepsilon + V(x)\psi_j^\varepsilon + W(x,t)\psi_j^\varepsilon \quad \text{(High frequency)};$$
$$i\varepsilon\partial_t \psi_j^\varepsilon = -\tfrac{1}{2}\varepsilon^2 \Delta \psi_j^\varepsilon + V(x)\psi_j^\varepsilon + W(x,t)\psi_j^\varepsilon \quad \text{(Low frequency)},$$

where $V = V_c + V_{xc}$.

Crystals - periodicity assumptions

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- Assume the external potential W is 1-periodic in x.
- The unit cell is ε-periodic and contains N electron.

Then

$$-\varepsilon^2 \Delta V_c = \varepsilon^3(\rho^\varepsilon - m^\varepsilon), \quad V_{xc} = \eta(\varepsilon^3 \rho^\varepsilon),$$

where

$$\rho^\varepsilon = \sum_{j=1}^{Z\varepsilon^{-3}} \left|\psi_j^\varepsilon\right|^2, \quad m^\varepsilon = \varepsilon^{-3} m(x/\varepsilon).$$

High frequency regime - short time dynamics

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$$\begin{cases} i\partial_t \psi_j^\varepsilon = -\frac{1}{2}\varepsilon^2 \Delta \psi_j^\varepsilon + V(x,t)\psi_j^\varepsilon + W(x,t)\psi_j^\varepsilon, \\ -\varepsilon^2 \Delta V_c = \varepsilon^3(\rho^\varepsilon - m^\varepsilon), \quad V_{xc} = \eta(\varepsilon^3 \rho). \end{cases}$$

Denote $V_{tot} = V + W$.

Remark that $\rho^\varepsilon = \sum^{Z\varepsilon^{-3}} \left|\psi_j^\varepsilon\right|^2 \sim O(1/\varepsilon^3)$.

Assume initially the system is at the ground state $\rho^\varepsilon(x,0) = \varepsilon^{-3}\rho_0(x/\varepsilon)$ of the unperturbed system ($W = 0$).

Interested in: macroscopic response in V to W as $\varepsilon \to 0$.

Band structure

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Denote the Hamiltonian for the unperturbed system (in a.u.)

$$H_0 = -\frac{1}{2}\Delta + V_{\text{per}} \quad \text{with} \quad -\Delta V_{\text{per}} = \rho_0 - m.$$

Bloch-Floquet theory shows

$$H_0 = \fint_{\Gamma^*} H_{0,\boldsymbol{k}}\,\mathrm{d}\boldsymbol{k} = \fint_{\Gamma^*} \sum_n E_n(\boldsymbol{k})|\psi_{n,\boldsymbol{k}}\rangle\langle\psi_{n,\boldsymbol{k}}|\,\mathrm{d}\boldsymbol{k}.$$

$\psi_{n,\boldsymbol{k}}$ and $E_n(\boldsymbol{k})$ are the eigenfunctions and eigenvalues (sorted in increasing order) of $H_{0,\boldsymbol{k}}$. $\psi_{n,\boldsymbol{k}} = u_{n,\boldsymbol{k}} \exp(i\boldsymbol{k}\cdot\boldsymbol{x})$.

Band gap assumption:

The first Z bands are occupied with a gap from the others.

Main results

$$V_{tot}(t,x) = \big(V_{per}(x/\varepsilon) + U_0(t,x)\big) + \mathcal{O}(\varepsilon),$$

where U_0 satisfies,

$$-\Delta_x U_0(t,x) - \int_0^t G(t-\tau) : \nabla_x^2 U_0 \,\mathrm{d}\tau = -\Delta_x W(t,x),$$

and

$$G(t) = \frac{1}{2\pi}\int e^{-i\omega t} G(\omega)\,\mathrm{d}\omega.$$

A physically more clear form:

$$-\Delta_x \widehat{U_0}(\omega,x) - G(\omega) : \nabla_x^2 \widehat{U_0}(\omega,x) = -\Delta_x \widehat{W}(\omega,x).$$

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$G(\omega)$ is determined by the band structure

$$G_{\alpha\beta}(\omega) = \sum_{n\leq Z}\sum_{m>Z} \fint_{\Gamma^*} \mathfrak{Re}\frac{\overline{\langle u_{n,\boldsymbol{k}}|i\partial_{\boldsymbol{k}_\alpha}|u_{m,\boldsymbol{k}}\rangle}\langle u_{n,\boldsymbol{k}}|i\partial_{\boldsymbol{k}_\beta}|u_{m,\boldsymbol{k}}\rangle}{\omega+\omega_{mn}(\boldsymbol{k})}\,\mathrm{d}\boldsymbol{k}$$

$$- \sum_{n\leq Z}\sum_{m>Z} \fint_{\Gamma^*} \mathfrak{Re}\frac{\overline{\langle u_{n,\boldsymbol{k}}|i\partial_{\boldsymbol{k}_\alpha}|u_{m,\boldsymbol{k}}\rangle}\langle u_{n,\boldsymbol{k}}|i\partial_{\boldsymbol{k}_\beta}|u_{m,\boldsymbol{k}}\rangle}{\omega-\omega_{mn}(\boldsymbol{k})}\,\mathrm{d}\boldsymbol{k}$$

$$- \left\langle f_{\omega,\alpha}, \mathcal{V}(1-\chi_\omega\mathcal{V})^{-1} f_{\omega,\beta}\right\rangle,$$

$$\omega_{mn} = E_m(\boldsymbol{k}) - E_n(\boldsymbol{k}).$$

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The function f and operator χ_ω from δV to $\delta\rho$,

$$f_{\omega,\alpha} = -\sum_{n\le Z}\sum_{m>Z} \fint_{\Gamma^*} \frac{u_{n,\boldsymbol{k}} u^*_{m,\boldsymbol{k}}}{\omega+\omega_{mn}(\boldsymbol{k})} \langle u_{n,\boldsymbol{k}}|i\partial_{\boldsymbol{k}_\alpha}|u_{m,\boldsymbol{k}}\rangle \,\mathrm{d}\boldsymbol{k}$$
$$+\sum_{n\le Z}\sum_{m>Z} \fint_{\Gamma^*} \frac{u^*_{n,\boldsymbol{k}} u_{m,\boldsymbol{k}}}{\omega-\omega_{mn}(\boldsymbol{k})} \overline{\langle u_{n,\boldsymbol{k}}|i\partial_{\boldsymbol{k}_\alpha}|u_{m,\boldsymbol{k}}\rangle} \,\mathrm{d}\boldsymbol{k},$$

$$\chi_\omega g = -\sum_{n\le Z}\sum_{m>Z} \fint_{\Gamma^*} \frac{u_{n,\boldsymbol{k}} u^*_{m,\boldsymbol{k}}}{\omega+\omega_{mn}(\boldsymbol{k})} \langle u_{n,\boldsymbol{k}}|g|u_{m,\boldsymbol{k}}\rangle \,\mathrm{d}\boldsymbol{k}$$
$$+\sum_{n\le Z}\sum_{m>Z} \fint_{\Gamma^*} \frac{u^*_{n,\boldsymbol{k}} u_{m,\boldsymbol{k}}}{\omega-\omega_{mn}(\boldsymbol{k})} \overline{\langle u_{n,\boldsymbol{k}}|g|u_{m,\boldsymbol{k}}\rangle} \,\mathrm{d}\boldsymbol{k}.$$

The linear map from $\delta\rho$ to δV,

$$\mathcal{V}h = \phi + \eta'(\rho_{per})h,$$
$$-\Delta_z\phi = h.$$

Discussions on short time dynamics

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- Microscopic justification of the effective Poisson equation in crystals (semiconductors or insulators).
- The external could be viewed as generated by free charge $-\Delta W$, then $\mathcal{E} = I + G$ gives the dielectric response (permittivity) tensor.
- The limit of $\omega \to 0$ recovers the static dielectric response (Baroni-Resta, 1986), recently rigorously studied by Cancés-Lewin (2010) in the linear response regime.

Asymptotics

$$\rho = \varepsilon^{-3}\rho_0(t,x,x/\varepsilon) + \varepsilon^{-2}\rho_1(t,x,x/\varepsilon) + \varepsilon^{-1}\rho_2(t,x,x/\varepsilon) + \cdots$$

$$V_{\mathrm{tot}}(t,x) = V_0(t,x,x/\varepsilon) + \varepsilon V_1(t,x,x/\varepsilon) + \varepsilon^2 V_2(t,x,x/\varepsilon) + \cdots$$

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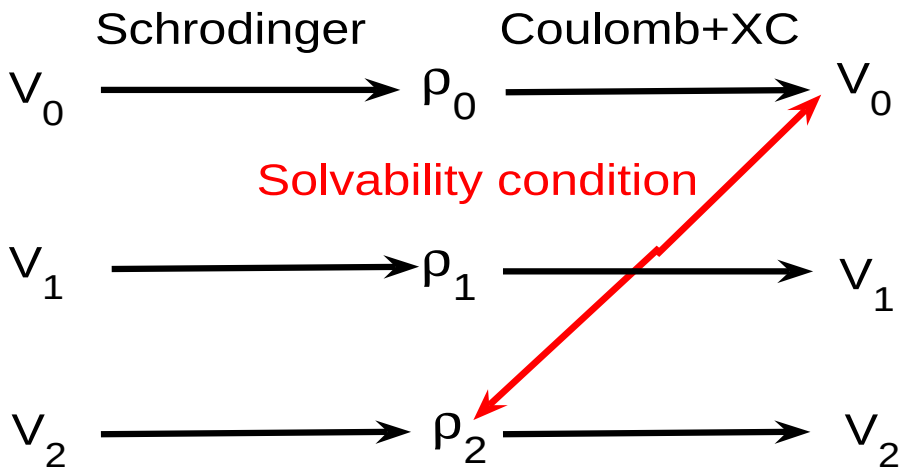

Two scaled Coulomb equation, $z = x/\varepsilon$,

$$-\Delta_z V_\ell - 2\nabla_x \cdot \nabla_z V_{\ell-1} - \Delta_x V_{\ell-2} = \rho_\ell - \delta_{0\ell} m.$$

Solvability condition:

$$\langle \rho_0 \rangle = \langle m \rangle, \quad \langle \rho_1 \rangle = 0, \quad -\Delta_x \langle V_0 \rangle = \langle \rho_2 \rangle.$$

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Heisenberg's picture:

$$\mathcal{P}_t^\varepsilon = \mathcal{T}\exp\left(-i\int_0^t H^\varepsilon(\tau)\right)\mathcal{P}_0^\varepsilon\left(\mathcal{T}\exp\left(-i\int_0^t H^\varepsilon(\tau)\right)\right)^*,$$

$$\rho^\varepsilon(t,x) = \mathcal{P}_t^\varepsilon(x,x),$$

Key observation:

The domain of dependence and influence in the evolution is of scale of cell size $\mathcal{O}(\varepsilon)$.

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$$\mathcal{H}_0(t,x) = -\frac{\varepsilon^2}{2}\Delta_y + V_0(t,x,y/\varepsilon),$$

$$\delta\mathcal{H}_1^\varepsilon(t,x) = (y-x)\cdot\nabla_x V_0(t,x,y/\varepsilon) + \varepsilon V_1(t,x,y/\varepsilon),$$

$$\delta\mathcal{H}_2^\varepsilon(t,x) = \frac{1}{2}\big((y-x)\cdot\nabla_x\big)^2 V_0(t,x,y/\varepsilon) + \varepsilon(y-x)\cdot\nabla_x V_1(t,x,y/\varepsilon) + \varepsilon^2 V_2(t,x,y/\varepsilon).$$

$$\begin{aligned}
&\mathcal{T}\exp(-i\int_0^t \mathcal{H}^\varepsilon(\tau)) \\
=&\mathcal{U}_{t,0}(x_0) - i\int_0^t \mathcal{U}_{t,\tau}(x_0)\delta\mathcal{H}^\varepsilon(\tau,x_0)\mathcal{U}_{\tau,0}(x_0)\,\mathrm{d}\tau \\
&- \int_0^t\int_0^{\tau_2} \mathcal{U}_{t,\tau_2}(x_0)\delta\mathcal{H}^\varepsilon(\tau_2,x_0)\mathcal{U}_{\tau_2,\tau_1}(x_0) \\
&\qquad\times\delta\mathcal{H}^\varepsilon(\tau_1,x_0)\mathcal{U}_{\tau_1,0}(x_0)\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2 + \cdots,
\end{aligned}$$

$$\mathcal{U}_{t,s}(x_0) = \mathcal{T}\exp(-i\int_s^t \mathcal{H}_0(\tau,x_0)\,\mathrm{d}\tau).$$

Low frequency regime - long time dynamics

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$$\begin{cases} i\varepsilon\partial_t\psi_j^\varepsilon = -\frac{1}{2}\varepsilon^2\Delta\psi_j^\varepsilon + V(x)\psi_j^\varepsilon + W(x,t)\psi_j^\varepsilon, \\ -\varepsilon^2\Delta V = \varepsilon^3(\rho^\varepsilon - m^\varepsilon). \end{cases}$$

Simplifications:

- No exchange correlation potential;
- Assume we only have valance and conduction bands;
- initially the system is at the ground state of the unperturbed system ($W = 0$).

Interested in: derivation of mesoscopic transport equations.

Two species transport equations

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$$\begin{cases} \text{Homogenized system:} \\ \partial f_{1,k}^{v,c} + \nabla_k E_{v,c} \cdot \nabla_x f_{1,k}^{v,c} = \mathcal{K}^{v,c} : \nabla_x q_{1,k}^{v,c} + h^{v,c}(\nabla_x v_1), \\ \partial_t q_{1,k}^{v,c} + \nabla_k E_{v,c} \cdot \nabla_x q_{1,k}^{v,c} + \nabla_x (v_1 + \langle V_1 \rangle) = 0, \\ \text{cell problem:} \\ (-\Delta_z + \mathcal{R}) v_1 = \fint_{\Gamma^*} (f_{1,k}^v |\chi_v|^2 + f_{1,k}^c |\chi_c|^2) + g^v + g^c \, \mathrm{d}k. \end{cases}$$

Incompressibility condition: $\langle \rho_1 \rangle = \fint f_{1,k}^v + f_{1,k}^c \, \mathrm{d}k = 0.$

- For each species, we have equations for the density $f_{1,k}^{v,c}$ and current $q_{1,k}^{v,c}$, interacted by $\mathcal{K}^{v,c}$ (given later).
- The interaction of these two species is through the microscopic potential v_1.

Discussions on long time dynamics

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- $\langle V_1 \rangle$ serves as the Lagrangian multiplier.
- The closure strategy is different from the short time dynamics. The response macroscopic potential serves as the Lagrange multiplier.
- Why interested in the first order system? The number density is of order ε^{-2}. If we try to recover the physical system and take $\varepsilon = 10^{-10}$, then the total charge density is roughly of $\mathcal{O}(1)$.
- If the initial conditions are zero, the system has (trivial) solutions (zero). This is consistent with the fact that a pure insulator does not conduct electricity. To make a semiconductor, we need to disturb the system so that the initial conditions of the first order system are nonzero. For example, p-n junction.

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$$\psi_k = \varepsilon^{-3/2}\psi_{0,k}(t,x,x/\varepsilon) + \varepsilon^{-1/2}\psi_{1,k}(t,x,x/\varepsilon) + \varepsilon^{1/2}\psi_{2,k}(t,x,x/\varepsilon) + \cdots$$

$$V(t,x) = V_0(t,x,x/\varepsilon) + \varepsilon V_1(t,x,x/\varepsilon) + \varepsilon^2 V_2(t,x,x/\varepsilon) + \cdots$$

Two scaled Coulomb equation, $z = x/\varepsilon$,

$$-\Delta_z V_\ell - 2\nabla_x \cdot \nabla_z V_{\ell-1} - \Delta_x V_{\ell-2} = \rho_\ell - \delta_{0\ell} m.$$

Constraints:

$$\langle \rho_0 \rangle = \langle m \rangle, \quad \langle \rho_1 \rangle = 0, \quad -\Delta_x \langle V_0 \rangle = \langle \rho_2 \rangle.$$

WKB analysis

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$$\psi_{0,k}(t,x,z) = \varphi_{0,k}(t,x,z)\exp(iS_k(t,x)/\varepsilon).$$

Adiabatic approx. $\varphi_{0,k}(t,x,z) = a_{0,k}(t,x)\chi_n(\nabla_x S_k, z).$

$$\mathcal{H}\chi_n = \left(\frac{1}{2}(-i\nabla_z + p)^2 + V_{per}(z)\right)\chi_n(p,z) = E_n(p)\chi_n(p,z).$$

Valence band: $a^v_{0,k}(t,x) = 1, S^v_k(0,x) = kx$ (full band)

Conduction band: $a^c_{0,k}(t,x) = 0, S^c_k(0,x) = kx$ (empty band)

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To the leading order, one gets eikonal-transport equations,

$$\partial_t S_k^{v,c} + E_{v,c}(\nabla_x S_k^{v,c}) = 0 \quad (\Rightarrow) \quad S_k^{v,c}(t,x) = kx - E_{v,c}(k)t,$$

$$\partial_t a_{0,k}^{v,c} + \nabla_k E_{v,c}(k) \cdot \nabla_x a_{0,k}^{v,c} + i a_{0,k}^{v,c}(v_1 + \langle V_1 \rangle) = 0,$$

$$\left|a_{0,k}^{v}\right|^2 = 1, \quad \left|a_{0,k}^{c}\right|^2 = 0,$$

$$\langle \rho_0 \rangle = \int \left|a_{0,k}^{v}\right|^2 + \left|a_{0,k}^{c}\right|^2 \, \mathrm{d}k = \langle m \rangle .$$

This fulfills the behavior of insulator: although each electron has classical dynamics

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \nabla_k E_{v,c},$$

it does not conduct electricity. It proposes a constraint

$$\langle V_0 \rangle + W = 0, \quad \langle \rho_2 \rangle = \Delta_x W$$

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The first order correction. Assume

$$\psi_{1,k}^{v,c}(t,x,z) = a_{1,k}^{v,c}\chi_{v,c}(k,z) + \left(\varphi_{1,k}^{v,c}\right)^{\perp}.$$

Define

$$f_{1,k}^{v,c} = 2\mathfrak{Re}\left\langle \left(\psi_{0,k}^{v,c}\right)^{*}\psi_{1,k}^{v,c}\right\rangle, \quad q_{1,k}^{v,c} = \mathfrak{Im}\left\langle \left(\psi_{0,k}^{v,c}\right)^{*}\nabla_x\psi_{0,k}^{v,c}\right\rangle.$$

then

$$\mathcal{K}_{\alpha\beta}^{v,c} = 2\mathfrak{Re}\langle \partial_{z_\alpha}\chi_{v,c}, \mathcal{L}_{v,c}^{-1}(I-\mathcal{P}^{v,c})\partial_{z_\beta}\chi_{v,c}\rangle - \delta_{\alpha\beta},$$

$$\mathcal{L}_{v,c} = \mathcal{H} - E_{v,c},$$

$$h^{v,c}(\nabla_x v_1) = -2\mathfrak{Im}\langle \nabla_z\chi_{v,c}, \mathcal{L}_{v,c}^{-1}(I-\mathcal{P}^{v,c})(\nabla_x v_1\chi_{v,c})\rangle,$$

$$\mathcal{R}v_1 = 2\fint \mathfrak{Re}\left(\chi_{v,c}^{*}\mathcal{L}_{v,c}^{-1}(v_1\chi_{v,c})\right),$$

$$g^{v,c} = -2\fint_{\Gamma^*} \mathfrak{Im}\left(\chi_{v,c}^{*}\mathcal{L}_{v,c}^{-1}(I-\mathcal{P}^{v,c})\nabla_z\chi_{v,c}\right)\cdot q_{1,k}^{v,c}\,\mathrm{d}k.$$

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Homogenized system - high frequency regime

Homogenized systems - low frequency regime

Conclusions:

- We derive the Thomas-Fermi-Maxwell model and study the half space problem.
- Effective dielectric response equation is derived in the high frequency regime of the Kohn-Sham model.
- Effective transport equations are derived in the low frequency regime of the Kohn-Sham model.

Future work:

- More realistic models in surface plasmon and semiconductor.For example, the grating surface and p-n junction.
- Electron dynamics in the presence of magnetic field.

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Thank You!

Questions?