Some topics on quantum transport

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Overview

Study quantum transport within density functional theory.

- Junction of two 1-d embedded in 3d periodic systems. (A warming up problem)
- Quantum transport : i.e., conductivity etc.
- Coupling with phonons (Extension of Thomas- Fermi -von Weizsäcker model)

Other interesting topics :

- Topological insulators, bulk-edge correspondence, Quantum Hall Effect, etc.

- $\mathfrak{H}$: a separable Hilbert space (usually used : $L^2(\mathbb{R}^3)$, $H^1(\mathbb{R}^3)$) with $(\psi_i)_{i=1}^{\infty}$ as orthogonal basis.
- $\mathcal{L}(\mathfrak{H})$: bounded operator on $\mathfrak{H}$.
- For $A \in \mathcal{L}(\mathfrak{H})$ which is **positive**, define its trace:

$$\mathrm{Tr}(A) := \sum_{i=1}^{\infty} (\psi_i, A\psi_i).$$

For Probabilists, please consider this as some form of expectation of some r.v.

- Schatten class $\mathfrak{S}^p(\mathfrak{H})$ (Non-commutative L^p space) :

$$A \in \mathfrak{S}^p(\mathfrak{H}) \Longleftrightarrow \mathrm{Tr}\left(|A|^p\right)^{1/p} < \infty, \qquad |A| = \sqrt{A^*A} \tag{1}$$

- A is in trace-class $\Longleftrightarrow A \in \mathfrak{S}_1(\mathfrak{H})$, A is in Hilbert-Schmidt $\Longleftrightarrow A \in \mathfrak{S}_2(\mathfrak{H})$.

Motivation: study the junction of two 1-d embeded in 3d periodic systems with reduced Hartree-Fock model.

- Calculate its ground state $\rightarrow$ minimization of energy functional.
- Existence of ground state $\rightarrow$ existence of minimizer of energy functional.

For N nonrelativistic quantum electrons, reduced Hartree-Fock model is a mean-field model

- the state of N electrons described by one-body density matrix γ, where $\gamma \in \mathcal{P}^N$:

$$\mathcal{P}^N = \left\{ \gamma \in \mathcal{B}(L^2(\mathbb{R}^3)) \mid 0 \leq \gamma \leq 1, \mathrm{Tr}(\gamma) = N, \mathrm{Tr}\left(\sqrt{-\Delta}\gamma\sqrt{-\Delta}\right) < \infty \right\}$$

- N-body space of fermionic wavefunctions : $\wedge_{i=1}^N H^1(\mathbb{R}^3)$.
- Hartree-Fock state : $\Phi := \psi_1 \wedge \psi_2 \wedge \cdots \wedge \psi_N \in \wedge_{i=1}^N H^1(\mathbb{R}^3)$.
- $\gamma = \sum_{i=1}^N |\psi_i\rangle \langle\psi_i|$ density matrix of $\Phi \rightarrow$ diagonalizable in an orthogonal basis $(\phi_i)_{i=1}^\infty$ of $L^2(\mathbb{R}^3)$: $\gamma = \sum_{i=1}^\infty n_i |\phi_i\rangle \langle\phi_i|$, $0 \leq n_i \leq 1$.
- Density associated with γ: $\rho_\gamma(x) = \gamma(x,x) = \sum_{i=1}^\infty n_i \phi_i^2(x) \geq 0$.

- Nuclei density of charge $\rho_{\rm nuc}$.
- reduced Hartree-Fock energy functional :

$$\mathcal{E}^{\rm rHF}(\gamma) = {\rm Tr}\left(-\frac{1}{2}\gamma\right) + \frac{1}{2}D\left(\rho_\gamma - \rho_{\rm nuc}, \rho_\gamma - \rho_{\rm nuc}\right). \qquad (2)$$

$$D(f,g) = \int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x)g(y)}{|x-y|}dxdy = 4\pi\int_{\mathbb{R}^3} \frac{\overline{\hat{f}(k)}\hat{g}(k)}{|k|^2}dk.$$

- The variational problem is :

$$I_{rHF} = \inf\left\{\mathcal{E}^{\rm rHF}(\gamma), \gamma\in\mathcal{P}^N\right\}$$

Theorem : for neutral or positively charged systems, the variational problem has a minimizer γ and ρ_γ is unique .

Bloch decomposition for 1d embedded in 3d periodic infinite system:

- Unit cell: $\Gamma := [-1/2, 1/2) \times \mathbb{R}^2$.
- The first Brillouin zone (dual lattice): $\Gamma^* := [-\pi, \pi) \times \{0\}^2 \equiv [-\pi, \pi)$
- Translation operator : $\tau_k u(x, \boldsymbol{r}) = u(x - k, \boldsymbol{r}), \forall k \in \mathbb{R}$
- Density matrix of the electrons: γ, which is a self-adjoint operator acting on $L^2(\mathbb{R}^3)$ and $0 \leq \gamma \leq 1$.
- Bloch decomposition:

$$L^2_\xi(\Gamma) = \left\{ u \in L^2_{\mathrm{loc}}(\mathbb{R}, L^2(\mathbb{R}^2)) \mid \tau_k u = e^{-ik\xi} u, \forall k \in \mathbb{Z} \right\}$$

$$\gamma = \frac{1}{2\pi} \int_{\Gamma^*} \gamma_\xi d\xi, \quad \gamma_\xi \in \mathcal{S}(L^2_\xi(\Gamma))$$

We can define a 1d embeded in 3d periodic rHF energy for $\gamma \in \mathcal{P}_{\rm per}$:

$$\boxed{\mathcal{E}_{\rm per}(\gamma) = \frac{1}{2\pi}\int_{\Gamma^*} \mathrm{Tr}_{L^2_\xi(\Gamma)}\left(-\frac{1}{2}\Delta\gamma_\xi\right) d\xi + \frac{1}{2} D_G(\rho_\gamma - \mu_{\rm per}, \rho_\gamma - \mu_{\rm per})} \qquad (3)$$

The periodic rHF ground state energy (per unit cell) is given by

$$\boxed{I_{\rm per} = \inf\left\{\mathcal{E}_{\rm per}(\gamma), \gamma \in \mathcal{P}_{\rm per}, \int_\Gamma \rho_\gamma = Z\right\}} \qquad (4)$$

$$D_G(f,g) := \int_\Gamma \int_\Gamma G(\boldsymbol{x} - \boldsymbol{y}) f(\boldsymbol{x}) g(\boldsymbol{y}) d\boldsymbol{x} d\boldsymbol{y}$$

ρ_γ: density associate with γ.
$G(\cdot)$: Green function

Theorem

(Definition of the 1d periodic rHF minimizer) Let $Z \in \mathbb{N}\backslash\{0\}$*. The minimization problem (4) admits a unique minimizer* $\gamma_{\rm per}$*. Moreover,* $\gamma_{\rm per}$ *satisfies the following self-consistent equation:*

$$\begin{cases} \gamma_{\rm per} = \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\rm per}) \\ H_{\rm per} := -\frac{1}{2}\Delta + (\rho_{\rm per} - \mu_{\rm per}) \star_\Gamma G \end{cases} \tag{5}$$

where ϵ_F *is a Lagrange multiplier called Fermi level (chemical potential).*

Difficulty: if not the same periodicity, there is breaking translation symmetry $\rightarrow$ Bloch decomposition cannot be applied $\rightarrow$ need to find a reference state.

- Periodic density operator corresponding to the left (right) system: $\gamma_{\mathrm{per},\ell}$ ($\gamma_{\mathrm{per},r}$) solution of (5), with nuclei density $\mu_{\mathrm{per},\ell}$ ($\mu_{\mathrm{per},r}$) and electronic density $\rho_{\mathrm{per},\ell}$ ($\rho_{\mathrm{per},r}$).
- Density operator of junction system: γ_s, with associated density ρ_s.
- $\mu_s = \mathbb{1}_{x\leq 0} \cdot \mu_{\mathrm{per},\ell} + \mathbb{1}_{x\geq 0} \cdot \mu_{\mathrm{per},r} \quad , \quad D(f,g) := 4\pi \int_{\mathbb{R}^3} \frac{\overline{\hat{f}(k)}\hat{g}(k)}{k^2} dk.$
- (Infinite) energy functional for the junction system is FORMALLY:

$$\mathcal{E}_s(\gamma_s) := \mathrm{Tr}\left(-\frac{1}{2}\Delta\gamma_s\right) + \frac{1}{2}D(\rho_s - \mu_s, \rho_s - \mu_s) \tag{6}$$

Objective: find a reference state γ_r, and perturbative state Q, such that $\gamma_s = \gamma_r + Q$.

Choice of reference state γ_r :

- Need to be an orthogonal spectral projector of some well-chosen Hamiltonian, i.e., $0 \leq \gamma_r \leq 1$, $\gamma_r^2 = \gamma_r$ and $\gamma_r^* = \gamma_r$. (If not we do not know yet how to treat its perturbation ...)
- Need to have enough regularity (Laplacian term ...)
- Need to approach the real state γ_s such that the difference can be treated as perturbation (Very logic !)

$\rightarrow$ should be something that is very similar to $\mathbb{1}_{x \leq 0} \cdot \gamma_{\text{per},\ell} + \mathbb{1}_{x \geq 0} \cdot \gamma_{\text{per},r}$. (Not this one, lack of regularity, the smooth version is not a spectral projector of some Hamiltonian ...)

Choice of reference state

- Introduce a smooth function $\chi(x, y, z)$:

$$\chi(x,\cdot,\cdot) = \begin{cases} 1 & \text{if } x \leq -1/2 \\ 0 & \text{if } x \geq 1/2 \\ \text{smooth elsewhere, bounded between 0 and 1} \end{cases} \tag{7}$$

- A regular potential $V_\chi := \chi^2 V_{\mathrm{per},\ell} + (1-\chi^2) V_{\mathrm{per},r} = \chi^2 \left((\rho_{\mathrm{per},\ell} - \mu_{\mathrm{per},\ell}) \star_\Gamma G\right) + (1-\chi^2)\left((\rho_{\mathrm{per},r} - \mu_{\mathrm{per},r}) \star_\Gamma G\right)$.
- Define Hamiltonian associated with V_χ writes:

$$\boxed{H_\chi := -\frac{1}{2}\Delta + V_\chi} \tag{8}$$

- Define a spectral projector

$$\gamma_r = \gamma_\chi := \mathbb{1}_{(-\infty,\epsilon_F]}(H_\chi)$$

we have $[\gamma_\chi, H_\chi] = 0$.

- $\rho_\chi - \mu_\chi := -\frac{1}{4\pi}\Delta V_\chi = \left(\chi^2(\rho_{\mathrm{per},\ell} - \mu_{\mathrm{per},\ell}) + (1-\chi^2)(\rho_{\mathrm{per},r} - \mu_{\mathrm{per},r})\right) + \eta_\chi$. η_χ is local term.
- ρ_χ and is *a priori* unknown, is decided by $\rho_\chi := \mathbb{1}_{(-\infty,\epsilon_F]}(H_\chi)$.
- Perturbative energy

$$\mathcal{E}_s(\gamma_s) - \mathcal{E}_r(\gamma_r) \overbrace{=}^{\text{formally}} \mathrm{Tr}\left(-\frac{1}{2}\Delta Q\right) + D(\rho_\chi - \mu_\chi, \rho_Q) + \frac{1}{2}D(\rho_Q, \rho_Q) - D(\rho_Q, \nu_\chi) - D(\rho_\chi - \mu_\chi, \nu_\chi) + \frac{1}{2}D(\nu_\chi, \nu_\chi) \tag{9}$$

where

$$\nu_\chi := \mu_s - \mu_\chi = (\mathbb{1}_{x\le 0} - \chi^2)\mu_{\mathrm{per},\ell} + (\mathbb{1}_{x\ge 0} - (1-\chi^2))\mu_{\mathrm{per},r} + (\chi^2\rho_{\mathrm{per},\ell} + (1-\chi^2)\rho_{\mathrm{per},r} - \rho_\chi) + \eta_\chi \tag{10}$$

Objective: study the rigorous version of minimization problem (9).

Proposition (Reference state density is exponentially close to the smoothed real density)

Assume that Fermi level $\epsilon_F < 0$ (Fermi level is strictly negative), and a gap condition, we have $\chi^2\rho_{\mathrm{per},\ell} + (1-\chi^2)\rho_{\mathrm{per},r} - \rho_\chi \in \mathcal{C}\bigcap L^1(\mathbb{R}^3)\bigcap L^2(\mathbb{R}^3)$. So $\nu_\chi \in \mathcal{C}\bigcap L^1(\mathbb{R}^3)\bigcap L^2(\mathbb{R}^3)$. Moreover, denote $\mathcal{B}(Z)$ a unit cube centred at $Z \in \mathbb{Z}$, and $w(Z)$ the characteristic function of unit cube $\mathcal{B}(Z)$, there exists positive constants c_1, c_2 and m_1, m_2, and for $\alpha \in \mathbb{Z}^+$ and $\beta \in \mathbb{Z}$, such that

$$|\int_{\mathbb{R}} \left(\chi^2\rho_{\mathrm{per},\ell}(x,\cdot,\cdot) + (1-\chi^2)\rho_{\mathrm{per},r}(x,\cdot,\cdot) - \rho_\chi(x,\cdot,\cdot)\right) w(\beta)dx| \le c_1 e^{-m_1|\beta|},$$

$$|\int_{\mathbb{R}} \left(\chi^2\rho_{\mathrm{per},\ell}(\cdot,r,\cdot) + (1-\chi^2)\rho_{\mathrm{per},r}(\cdot,r,\cdot) - \rho_\chi(\cdot,r,\cdot)\right) w(\alpha)dr| \le c_2 e^{-m_2|\alpha|}.$$

Proof.

Write all in spectral projector form and use Cauchy formula representation, have norm estimations and by argument of duality to prove the result. □

Define $\mathfrak{S}_p$ by the Schatten class of operator acting on $L^2(\mathbb{R}^3)$ that have a finite p trace, i.e., $A \in \mathfrak{S}_p \Leftrightarrow \mathrm{Tr}(|A|^p) < \infty$. $p = 1$ ($p = 2$) is trace-class (Hilbert-Schmidt class).

- Q is not necessarily to be trace-class $\Rightarrow$ Definition of Π-trace class, Π an orthogonal projector.
- A self-adjoint compact operator A is said to be Π-trace class ($A \in \mathfrak{S}_1^{\Pi}$) if $A \in \mathfrak{S}_2$ and both $\Pi A \Pi$ and $(1 - \Pi)A(1 - \Pi)$ are in $\mathfrak{S}_1$.
- $\mathrm{Tr}_{\Pi}(Q) := \mathrm{Tr}(\Pi Q \Pi) + \mathrm{Tr}((1 - \Pi)Q(1 - \Pi))$

- Define a γ_χ-trace class:

$$\mathcal{Q}_\chi := \{Q \in \mathfrak{S}_1^{\gamma_\chi} \mid Q^* = Q,\ |\nabla|Q \in \mathfrak{S}_2,\ |\nabla|Q^{++}|\nabla| \in \mathfrak{S}_1,\ |\nabla|Q^{--}|\nabla| \in \mathfrak{S}_1\}$$

where $Q^{++} := (1-\gamma_\chi)Q(1-\gamma_\chi)$ and $Q^{--} := \gamma_\chi Q \gamma_\chi$. By construction, we have $\mathrm{Tr}_\chi(Q) = \mathrm{Tr}(Q^{++}) + \mathrm{Tr}(Q^{--})$.

- Define:

$$\boxed{\mathrm{Tr}_\chi(H_\chi Q) := \mathrm{Tr}(|H_\chi - \kappa|^{1/2}(Q^{++} - Q^{--})|H_\chi - \kappa|^{1/2}) + \kappa \mathrm{Tr}_\chi(Q)} \quad (11)$$

- Study the minimization problem of the following energy functional, which comes from the energy contribution containing Q in (9):

$$\boxed{\mathcal{E}_\chi(Q) := \mathrm{Tr}_\chi(H_\chi Q) - D(\rho_Q, \nu_\chi) + \frac{1}{2} D(\rho_Q, \rho_Q)} \quad (12)$$

Proposition (Definition of density ρ_Q for $Q \in \mathcal{Q}_\chi$)

For $Q \in \mathcal{Q}_\chi$, we have $QV \in \mathfrak{S}_1^{\gamma_\chi}$ for any $V = V_1 + V_2 \in \mathcal{C}' + L^2(\mathbb{R}^3)$. Moreover, there exists a constant c s.t. :

$$|\mathrm{Tr}_\chi(QV)| \leq c\|Q\|_{\mathcal{Q}_\chi}(\|V_1\|_{\mathcal{C}'} + \|V_2\|_{L^2(\mathbb{R}^3)})$$

Thus the linear form $V \in \mathcal{C}' + (L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)) \mapsto \mathrm{Tr}_\chi(QV)$ can be continuously extended to $\mathcal{C}' + L^2(\mathbb{R}^3)$ and there exists a uniquely defined function $\rho_Q \in \mathcal{C} + L^2(\mathbb{R}^3)$ such that

$$\forall V = V_1 + V_2 \in \mathcal{C}' + (L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)), \quad \langle \rho_Q, V_1 \rangle_{\mathcal{C}',\mathcal{C}} + \int_{\mathbb{R}^3} \rho_Q V_2 = \mathrm{Tr}_\chi(QV).$$

The linear map $Q \in \mathcal{Q}_\chi \mapsto \rho_Q \in \mathcal{C} \bigcap L^2(\mathbb{R}^3)$ is continuous :

$$\|\rho_Q\|_{\mathcal{C}} + \|\rho_Q\|_{L^2(\mathbb{R}^2)} \leq c\|Q\|_{\mathcal{Q}_\chi}$$

If $Q \in \mathfrak{S}_1 \in \mathfrak{S}_1^{\gamma_\chi}$, then $\rho_Q(x) = Q(x,x)$ where $Q(x,x)$ the integral kernel of Q.

Proposition (Energy functional is bounded from below)

Assume that gap condition holds, for $\kappa \in (\Sigma_Z^+, \Sigma_{Z+1}^-)$, there are constants d_1, d_2, such that

$$\mathcal{E}_\chi(Q) - \kappa \mathrm{Tr}_\chi(Q) \geq d_1 \Big(\|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1} + \||\nabla|Q^{++}|\nabla|\|_{\mathfrak{S}_1} + \||\nabla|Q^{--}|\nabla|\|_{\mathfrak{S}_1}$$
$$+ d_2 \Big(\||\nabla|Q\|_{\mathfrak{S}_2}^2 + \|Q\|_{\mathfrak{S}_2}^2 \Big) - \frac{1}{2} D(\nu_\chi, \nu_\chi).$$

Hence $\mathcal{E} - \kappa \mathrm{Tr}_\chi$ is bounded from below and coercive on $\mathcal{K}_\chi$. When $\nu_\chi \equiv 0$, $Q \mapsto \mathcal{E}_\chi(Q) - \kappa \mathrm{Tr}_\chi(Q)$ is non-negative, 0 being its unique minimizer.

Define an admissible set:

$$\mathcal{K}_\chi := \{Q \in \mathcal{Q}_\chi \mid -\gamma_\chi \le Q \le 1 - \gamma_\chi\}$$

Introduce the following minimization problem:

$$\boxed{E_{\epsilon_F,\chi} = \inf\{\mathcal{E}_\chi(Q) - \epsilon_F \mathrm{Tr}_\chi(Q), Q \in \mathcal{K}_\chi\}} \tag{13}$$

Proposition (Existence of minimizers with a chemical potential)

Assume that gap condition holds and $Z \in \mathbb{N}\backslash\{0\}$. Then:

- (Existence) For any $\epsilon_F \in (\Sigma_Z^+, \Sigma_{Z+1}^-)$, there exists a minimizer $\bar{Q}_\chi \in \mathcal{K}_\chi$ for (13). Problem (13) may have several minimizers, but they all share the same density $\bar{\rho}_\chi = \rho_{\bar{Q}_\chi}$. Any minimizer $\bar{Q}_\chi$ of (13) satisfies the self-consistent equation:

$$\begin{cases} \bar{Q}_\chi := \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\bar{Q}_\chi}) - \gamma_\chi + \delta \\ H_{\bar{Q}_\chi} = H_\chi + (\rho_{\bar{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1} \end{cases} \tag{14}$$

  where δ is a finite rank self-adjoint operator satisfying $0 \le \delta \le 1$ and $\mathrm{Ran}(\delta) \subseteq \mathrm{Ker}(H_{\bar{Q}_\chi} - \epsilon_F)$.

- (Regularity) Any $\bar{Q}_\chi \in \mathcal{K}_\chi$ solution of (14) belongs to $\mathcal{K}_{r,\chi}$.

Theorem (Independence of parameter)

$\rho_\chi + \rho_{Q_\chi}$ is independent of χ, where Q_χ is the solution of (14).

Theorem (Thermodynamic limit of the semi-infinite system)

$$\lim_{L\to\infty} I_{sc,L,s}(\gamma_{s_L}) - \mathcal{E}_{sc,L,\chi}(\gamma_{\chi_L}) = E_{\epsilon_F,\chi} - \int_{\mathbb{R}^3} \nu_\chi \left(\chi^2 V_{\mathrm{per}}\right) + \frac{1}{2} D(\nu_\chi, \nu_\chi)$$

Motivations : write a model for electrodes (modeled by 3d- infinite electron gaz) with mean-field Coulombian interactions.
Key words : Perturbation theory, Lieb-Thirring inequality, Hilbert space direct integral decomposition, etc ...

- Finite lattice, phonon dynamics coupling with Thomas-Fermi-von Weizsäcker model :

$$\begin{cases} -\Delta u(x,t) + u^{7/3}(x,t) - \Phi(x,t)u(x,t) = 0, \quad x \in \Gamma_N \\ u \geq 0 \\ -\Delta \Phi(x,t) = 4\pi\rho(x,t) := 4\pi \left(\sum_{k \in \mathcal{R}_N} \mu(x-k-q(k,t)) - u^2(x,t) \right) \\ m \dfrac{d^2 q(k,t)}{dt^2} = -\left(\nabla_x \Phi(x,t), \mu(x-k-q(k,t)) \right), \quad k \in \mathcal{R}_N \end{cases} \tag{15}$$

- Interesting questions for (15): is it well-posed ? global/local stability ? Extension to infinite lattice ? (Very difficult problem).