

Screening in the reduced Hartree–Fock model

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Joint work with Antoine Levitt (Université Paris-Saclay)
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Slides are online: jack.thomaslabs.co.uk/Herrsching

Electrostatic Screening: $\mu_{\text{def}} = Q\delta_0$

- Point charge in vacuum \Rightarrow long-range Coulomb potential
- In a material \Rightarrow material reorganises itself, total potential (Coulomb + response) is screened,
- Behaviour depends on whether charge carriers are mobile,
- Empirical models:

Vacuum

$$V(x) = v_c \mu_{\text{def}}(x)$$
$$= \frac{Q}{4\pi|x|},$$

Coulomb potential

Total screening

$$V(x) = \frac{Q}{4\pi|x|} e^{-k|x|}$$

Yukawa potential with screening length k^{-1}

Partial screening

$$V(x) = \frac{Q}{4\pi\varepsilon_r|x|}$$

Dielectric constant of the material $\varepsilon_r > 1$

Reduced Hartree–Fock (rHF) - finite systems

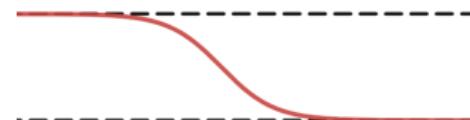
Coulomb operator:

$$v_c \rho(x) = \frac{1}{4\pi} \int \frac{\rho(y)}{|x - y|} dy$$

Potential-to-density:

$$\begin{aligned} F_{\varepsilon}(V)(x) &= f_{\varepsilon_F}(-\Delta + V)(x, x) \\ f_{\varepsilon_F}(x) &= (1 + e^{\frac{x - \varepsilon_F}{k_B T}})^{-1} \end{aligned}$$

Fermi–Dirac distribution:



Finite Systems

Total potential V satisfies:

$$V = V_{\text{ext}} + v_c F_{\varepsilon_F}(V)$$

$$\int_{\mathbb{R}^3} F_{\varepsilon_F}(V) = N_{\text{el}}$$

where: N_{el} – number of electrons,
 V_{ext} – external potential

k_B - Boltzmann const.

T - temperature

ε_F - Fermi level

- Hartree
- RPA
- Schrödinger–Poisson
- KSDFT w/o XC
- Hartree–Fock w/o exchange

Reduced Hartree–Fock (rHF)

$$\mathcal{E}(\gamma) = \text{Tr} \left(-\frac{1}{2} \Delta \gamma \right) + \int V_{\text{ext}} \rho_\gamma + \frac{1}{2} \int \rho_\gamma v_c \rho_\gamma$$

Convex variational problem

- existence γ and uniqueness ρ_γ
(neutral or positively charged systems)
[J-P Solovej, 1991]
- thermodynamic limit / periodic problem

[I. Catto, C. Le Bris, and P-L Lions, 2001]
[É. Cancès, A. Deleurence, and M. Lewin, 2008]

Finite Systems

Total potential V satisfies:

$$V = V_{\text{ext}} + v_c F_{\varepsilon_F}(V)$$

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N_{el} = # of electrons

V_{ext} = external potential

$$v_c \rho(x) = \frac{1}{4\pi} \int \frac{\rho(y)}{|x - y|} dy$$

$$F_\varepsilon(V)(x) = f_{\varepsilon_F}(-\Delta + V)(x, x)$$



Reduced Hartree–Fock (rHF)

$$\implies W_{\text{per}} = W_{\text{nucl}} + v_{\text{per}} F_{\varepsilon_F}(W_{\text{per}})$$

unique solution of the periodic rHF problem

Defect Problem

Change in potential V satisfies:

$$V = V_{\text{def}} + v_c(\rho_V - \rho_0)$$
$$\rho_V = F_{\varepsilon_F}(W_{\text{per}} + V)$$

Finte temperature: small defects are totally screened

[A. Levitt, 2020]

e.g. $V_{\text{def}} = \frac{Q}{|x|}$ for Q small enough,
 $V(V_{\text{def}})$ decays exponentially

Zero temperature: partial screening

[É. Cancès, M. Lewin, 2010]

Finite Systems

Total potential V satisfies:

$$V = V_{\text{ext}} + v_c F_{\varepsilon_F}(V)$$

$$\int_{\mathbb{R}^3} F_{\varepsilon_F}(V) = N_{\text{el}}$$

$N_{\text{el}} = \# \text{ of electrons}$

$V_{\text{ext}} = \text{external potential}$

$$v_c \rho(x) = \frac{1}{4\pi} \int \frac{\rho(y)}{|x - y|} dy$$

$$F_{\varepsilon}(V)(x) = f_{\varepsilon_F}(-\Delta + V)(x, x)$$

$$\begin{cases} -\Delta(v_{\text{per}} \rho) = \rho - \frac{1}{|\Gamma|} \int_{\Gamma} \rho \\ \int_{\Gamma} v_{\text{per}} \rho = 0 \end{cases}$$

Ideas in the proof

- Linearise: $V = V_{\text{def}} + v_c \chi_0 V$ and thus

$$V(V_{\text{def}}) = \varepsilon^{-1} V_{\text{def}} := (1 - v_c \chi_0)^{-1} V_{\text{def}}$$

where $\rho_V = \rho_0 + \chi_0 V + \dots$

- $\chi_{0,KK'}(q) := \langle e_K, \chi_{0,q} e_{K'} \rangle$ where $e_K := e^{iK \cdot x}$,
- For example, $K = K' = 0$

$$\begin{aligned}\chi_{0,00}(q) &\approx \sum_n \int_{\mathcal{B}} f'_{\varepsilon_F}(\varepsilon_{nk}) |u_{nk}|^2 dk + \sum_{n \neq m} \int_{\mathcal{B}} \frac{f_{\varepsilon_F}(\varepsilon_{nk}) - f_{\varepsilon_F}(\varepsilon_{mk})}{(\varepsilon_{n,k} - \varepsilon_{m,k})^3} |\langle q \cdot \nabla u_{mk}, u_{nk} \rangle|^2 dk \\ &= -\text{DOS} - q^T L q\end{aligned}$$

where $0 \leq L \in \mathbb{R}_{\text{sym}}^3$.

$$V = V_{\text{def}} + v_c (\rho_V - \rho_0)$$

Notation:

$$V = \int_{\mathcal{B}} V_q(x) e^{iq \cdot x} dq$$

$$AV = \int_{\mathcal{B}} (A_q V_q)(x) e^{iq \cdot x} dq$$

$$H_0 := -\Delta + W_{\text{per}}$$

$$H_{0,q} = \sum_n \varepsilon_{nq} |u_{nq}\rangle \langle u_{nq}|$$

more details

$$V(V_{\text{def}}) \approx \varepsilon^{-1} V_{\text{def}} = (1 - \nu_c \chi_0)^{-1} V_{\text{def}}$$

- Finite temperature: $\chi_0(q) \approx -\text{DOS}$ and $V_{\text{def}} = \frac{Q}{|x|}$, then

$$\hat{V}(q) = \frac{1}{1 + \frac{\text{DOS}}{|q|^2}} \frac{Q}{|q|^2} = \frac{Q}{|q|^2 + \text{DOS}} \quad \text{i.e.} \quad V = Q \frac{e^{-\sqrt{\text{DOS}}|x|}}{|x|}$$

- Insulators: $\chi_0(q) \approx -q^T L q$ and

$$\hat{V}(q) = \frac{1}{1 + \frac{q^T L q}{|q|^2}} \frac{Q}{|q|^2} = \frac{Q}{q^T M q} \quad \text{i.e.} \quad V = \frac{Q}{\sqrt{\det M}} \frac{1}{|x^T M^{-1} x|^{\frac{1}{2}}}$$

Metals at Zero Temperature

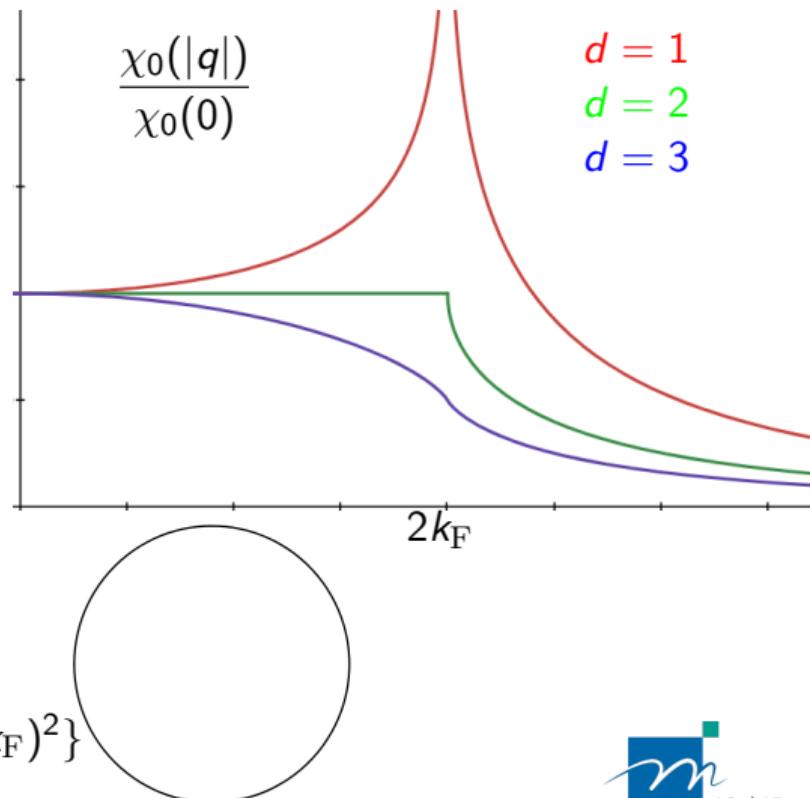
$$\chi_{0,00}(q) = \int_{\mathcal{B}} \frac{f_{\varepsilon_F}(\varepsilon_{k+q}) - f_{\varepsilon_F}(\varepsilon_k)}{\varepsilon_{k+q} - \varepsilon_k} |\langle u_k, u_{k+q} \rangle|^2 dk$$

Free electron gas, $\varepsilon_k = |k|^2$

$$V(V_{\text{def}}) \approx \varepsilon^{-1} V_{\text{def}} = (1 - v_c \chi_0)^{-1} \frac{Q}{|x|}$$
$$\sim Q \frac{\sin(2k_F|x| + (d-2)\frac{\pi}{2})}{|x|^d}$$

as $|x| \rightarrow \infty$.

$$\{k : \varepsilon_k = \varepsilon_F =: (k_F)^2\}$$



Metals at Zero Temperature

More generally,

$$\chi_0 V(x) = \frac{1}{\pi} \text{Im} \int_{-\infty}^{\varepsilon_F} \int_{\mathbb{R}^d} G_0(x, y; E) V(y) G_0(y, x; E) dy dE$$

where

$$G_0(x, y; E) := \lim_{\eta \downarrow 0} \int_{\mathcal{B}} \frac{u_k(x) u_k^*(y)}{E + i\eta - \varepsilon_k} e^{ik \cdot (x-y)} dk.$$

- Asymptotic behaviour of the Green's function
(contour deformation + stationary phase argument)
 \implies linear response behaviour

Friedel Oscillations in the reduced Hartree-Fock model

Jack Thorne. Joint work with Antonio Levitt.

Abstract. When a delta potential is placed in a domain, the material average and the local potential at the boundary change. This leads to oscillations in the energy levels. We study the case where the potential is supported by a small ball, and the ball is placed periodically. On the one hand, the energy levels at each point of the ball are periodic. On the other hand, the energy levels at the boundary are not necessarily periodic. In this talk, we will discuss how these two things interact, and define oscillations.

Introduction

Suppose we have a domain $\Omega \subset \mathbb{R}^d$ and a smooth potential V , we let $\{\lambda_j\}_{j=1}^\infty = \{\lambda_j(\Omega, V)\}$ be the eigenvalues of the Schrödinger operator $-\Delta + V$. For $k \in \mathbb{N}$ periods:

If a fixed potential $V(x) = \sum_{i=1}^k V_i(x)$ is constant on Ω_i , consider the response to an effect ϵ :

$$-\Delta + V_0 + \epsilon V_1 + \cdots + \epsilon V_k - \Delta + V_0 = \epsilon V_1 + \cdots + \epsilon V_k \quad (1)$$

where $V_i \in L^2(\Omega_i)$ is the i th component of the potential and V_0 is the constant potential. $T \geq 0$ and $\eta < 0$ is the independent particle scattering amplitude.

Linear model

$$\lambda_j = \lambda_j(\Omega, V) + \epsilon V_j \quad (2)$$

Particle temperature

$$\lambda_j = \lambda_j(\Omega, V) + \epsilon V_j \text{ where } V_j = V_j^*(V_0) \quad (3)$$

Dense temperature

$$\lambda_j = \lambda_j(\Omega, V) + \epsilon V_j \text{ where } V_j = V_j^*(V_0, \epsilon) \quad (4)$$

V_j oscillates and decays algebraically with ϵ depending on the surface $\partial\Omega_i$.

Group of the Green's Function

Non-interacting response goes in terms of the Green's function G :

$$G(x, y) = \frac{1}{4\pi} \int_{\partial\Omega} \int_{\partial\Omega} G_{ij}(x, y) d\sigma_i d\sigma_j \quad (5)$$

where

$$G_{ij} = \frac{\partial}{\partial x_i} G_{ij} = \frac{\partial}{\partial y_j} G_{ij} = -\frac{\partial}{\partial x_i} \frac{\partial}{\partial y_j} G_{ij} = -\frac{\partial}{\partial y_j} \frac{\partial}{\partial x_i} G_{ij} = \dots \quad (6)$$

In particular, we have

$$\begin{aligned} \partial_x G(x, y) &= \partial_y G(y, x) = \partial_x^2 G(x, y) = -\partial_y^2 G(y, x) = \dots \\ \partial_x^2 G(x, y) &= \partial_y^2 G(y, x) = \dots \end{aligned} \quad (7)$$

Therefore, the off-diagonal part of G has the corresponding type of decay for x_1 and $y_1 \sim \epsilon$.

A: Block diagonal with eigenvalues $\lambda_j = \lambda_j(\Omega, V) + \epsilon V_j^*(V_0)$ if $\Omega = \cup \Omega_i$ (Ω_i are k disjoint domains). $\lambda_j = \lambda_j(\Omega, V)$ if $\Omega = \Omega_0$ (Ω_0 is a single domain).

B: $\lambda_j = \lambda_j(\Omega, V) + \epsilon V_j$ where $V_j = V_j^*(V_0)$

Proposition 1: (Friedel's formula) Suppose that, at point $x \in \partial\Omega$ with normal in the direction ν , the surface $\partial\Omega$ has a hole of radius δ .

$$\lambda_j(x) = \lambda_j(\Omega, V) + \epsilon \sum_{i=1}^k \int_{\partial\Omega_i} G_{ij}(x, y) d\sigma_i \quad (8)$$

As $\epsilon \rightarrow 0$, $\lambda_j(x) \rightarrow \lambda_j(\Omega, V)$, where $\lambda_j(\Omega, V) = \lambda_j(\Omega \setminus \{x\}, V)$ are the principal eigenvalues of V on Ω .

Example: If $\Omega = \mathbb{R}^d$ has no periodic boundaries, we have $\lambda_j^2(\Omega) \leq C \epsilon^{-1}$. The main asymptotic behavior is then completely clear.

Figure 1: Decay of the Green's function for three model Fermi surfaces for $R = 1$, $\beta = 10$, $\alpha = 10$, $\gamma = 10$. The plots are together with point $x = (0, 0)$ and $y = (\sqrt{2}, 0)$. The plots are (a) circle, (b) ellipse, (c) figure-eight.

Sketch of the Proof. To quantify the decay, we take $\lambda_j = \lambda_j(\Omega, V)$ on $\Omega \setminus \{x\} = \Omega \setminus \{x_1, \dots, x_k\}$. Then,

$$\lambda_j^2(x) = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} G_{jj}(x, y) d\sigma_j d\sigma_j = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} [1 - G_{jj}(x, y)] d\sigma_j d\sigma_j \quad (9)$$

where $G_{jj} = \int_{\Omega \setminus \{x\}} G_{jj}(x, y) d\sigma_j$. We then apply stationary phase analysis to the oscillatory integral I :

Assumption: Particle Scattering $\epsilon \ll 1$ near resonance.

Result: For $x \in \Omega \setminus \{x\}$, define $\tilde{B} = \tilde{B}(x, \epsilon) = \epsilon^{-1/2}$ when $\tilde{B} > 1$ and $\tilde{B} = 1$ when $\tilde{B} \leq 1$. Then, for $y \in \Omega \setminus \{x\}$ with $|y - x| \leq \tilde{B}$, we have $\lambda_j^2(x) \leq C \epsilon^{-1}$ when $|y - x| \geq \tilde{B}$. The Fermi surface $\Omega \setminus \{x\}$ has ϵ -neighborhoods.

$$\lambda_j^2(x) = \epsilon^{-2} \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} G_{jj}(x, y) d\sigma_j d\sigma_j = \epsilon^{-2} \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} e^{i \epsilon^{-1/2} |x-y|} d\sigma_j d\sigma_j = \epsilon^{-2} \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} e^{i \epsilon^{-1/2} |x-y|} d\sigma_j d\sigma_j \quad (10)$$

as $|x-y| = o(\epsilon)$, where $d\sigma_j = d\sigma_j^{\text{osc}} + d\sigma_j^{\text{dc}}$ with $d\sigma_j^{\text{osc}} \ll d\sigma_j^{\text{dc}}$.

Remarks: By Proposition 1, we have $\lambda_j^2(x) = \epsilon^{-1}$ for $x \in \Omega$ with sufficient decay at infinity.

Figure 2: Decay of $\lambda_j^2(x)$ for the three model Fermi surfaces from Figure 1. $R = 1$, $\beta = 10$, $\alpha = 10$, $\gamma = 10$. The plots are together with setting $\epsilon = 1$ and $\alpha = 10$. The plots are (a) circle, (b) ellipse, (c) figure-eight.

Sketch of the Proof. Again, we obtain stability by controlling $\lambda_j^2(x) - \lambda_j^2(\Omega, V)$.

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When $\epsilon = 1/\tilde{B}$ we can switch to $\tilde{B} = 1/\epsilon$. Moreover, $\tilde{B} \ll 1$, $\tilde{B} = O(\epsilon)$. Therefore, one may use a partition of unity χ and integrate by parts to conclude.

Comments: A few remarks.

A: If finite temperature, $\rho_{ij} = \rho_{ji}$ unless $i = j$ and $\rho_{ii} = \rho_{ii}^{\text{dc}}$ which have form T^{-1} . This is a key difference between the Schrödinger operator and the Laplacian.

B: Assumptions are different. The theory is a bit easier.

C: We have made the effort to adapt the analysis to the exterior model $\Omega \setminus \{x\}$ for an additional approach involving writing down some precise estimates.

Under the same assumptions as Proposition 1: the discrete matrix $\langle \psi_j | \psi_j \rangle$ satisfies

$$\langle \psi_j | \psi_j \rangle = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} \langle \psi_j(x), \psi_j(y) \rangle d\sigma_j d\sigma_j = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} e^{i \epsilon^{-1/2} |x-y|} d\sigma_j d\sigma_j = \epsilon^{-2} \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} e^{i \epsilon^{-1/2} |x-y|} d\sigma_j d\sigma_j \quad (11)$$

A few words about the decay of $\langle \psi_j | \psi_j \rangle$ from the non-analytic behavior of the Lindhard function. $\langle \psi_j | \psi_j \rangle$ is finite. More complicated (multiple) Fermi surfaces.

Figure 3: Decay of the Green's function for four model Fermi surfaces for $R = 1$, $\beta = 10$, $\alpha = 10$, $\gamma = 10$. The plots are together with point $x = (0, 0)$ and $y = (\sqrt{2}, 0)$. The plots are (a) circle, (b) ellipse, (c) figure-eight, (d) leaf-like.

Sketch of the Proof. To quantify the decay, we take $\lambda_j = \lambda_j(\Omega, V)$ on $\Omega \setminus \{x\} = \Omega \setminus \{x_1, \dots, x_k\}$. Then,

$$\lambda_j^2(x) = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} G_{jj}(x, y) d\sigma_j d\sigma_j = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} [1 - G_{jj}(x, y)] d\sigma_j d\sigma_j \quad (12)$$

where $G_{jj} = \int_{\Omega \setminus \{x\}} G_{jj}(x, y) d\sigma_j$. We then apply stationary phase analysis to the oscillatory integral I :

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as $|x-y| = o(\epsilon)$, where $d\sigma_j = d\sigma_j^{\text{osc}} + d\sigma_j^{\text{dc}}$ with $d\sigma_j^{\text{osc}} \ll d\sigma_j^{\text{dc}}$.

Remarks: By Proposition 1, we have $\lambda_j^2(x) = \epsilon^{-1}$ for $x \in \Omega$ with sufficient decay at infinity.

Conclusion: Theorem 1.

Surfaces of revolution: $\Omega = \mathbb{R}^d$ with a smooth boundary $\partial\Omega$ and a smooth function $r(\theta)$ such that $\partial\Omega = \{r(\theta) \cos \theta, r(\theta) \sin \theta, h(\theta)\}$.

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as $|x-y| = o(\epsilon)$, where $d\sigma_j = d\sigma_j^{\text{osc}} + d\sigma_j^{\text{dc}}$ with $d\sigma_j^{\text{osc}} \ll d\sigma_j^{\text{dc}}$.

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as $|x-y| = o(\epsilon)$, where $d\sigma_j = d\sigma_j^{\text{osc}} + d\sigma_j^{\text{dc}}$ with $d\sigma_j^{\text{osc}} \ll d\sigma_j^{\text{dc}}$.

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$$\lambda_j^2(x) = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} G_{jj}(x, y) d\sigma_j d\sigma_j = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} [1 - G_{jj}(x, y)] d\sigma_j d\sigma_j = \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} e^{i \epsilon^{-1/2} |x-y|} d\sigma_j d\sigma_j = \epsilon^{-2} \int_{\Omega \setminus \{x\}} \int_{\Omega \setminus \{x\}} e^{i \epsilon^{-1/2} |x-y|} d\sigma_j d\sigma_j \quad (19)$$

as $|x-y| = o(\epsilon)$, where $d\sigma_j = d\sigma_j^{\text{osc}} + d\sigma_j^{\text{dc}}$ with $d\sigma_j^{\text{osc}} \ll d\sigma_j^{\text{dc}}$.

Remarks: By Proposition 1, we have $\lambda_j^2(x) = \epsilon^{-1}$ for $x \in \Omega$ with sufficient decay at infinity.

Conclusion: Theorem 1.

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Scattering Theory: Eigenfunction Expansions

- Want: $\rho_V - \rho_0$,

$$\rho_0(x) = f_{\varepsilon_F}(H_0)(x, x) = \int_{\mathcal{B}} f_{\varepsilon_F}(\varepsilon_k) |\Psi_k(x)|^2 dk$$

$$\rho_V(x) = \sum_{j: \lambda_j \leq \varepsilon_F} |\varphi_i(x)|^2 + \int_{\mathcal{B}} f_{\varepsilon_F}(\varepsilon_k) |\Psi_k^+(x)|^2 dk$$

- Idea: $\Psi_k^+ = \Omega^+ \Psi_k$ that “looks like” Ψ_k in the distant past:

$$\lim_{t \rightarrow -\infty} \left(e^{-iHt} \Psi_k^+ - e^{-iH_0 t} \Psi_k \right) = 0$$

- “ $\Omega^+ = \lim_{t \rightarrow -\infty} e^{iHt} e^{-iH_0 t}$ ”, $\Omega^+ H = H_0 \Omega^+$

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Proof

Notation:

$$H_0 = -\Delta + W_{\text{per}},$$

$$\Psi_k = u_k(x) e^{ik \cdot x} \text{ with}$$

$$H_0 \Psi_k = \varepsilon_k \Psi_k,$$

$$G_0(E) := (E + i0^+ - H_0)^{-1}$$

$$H = H_0 + V,$$

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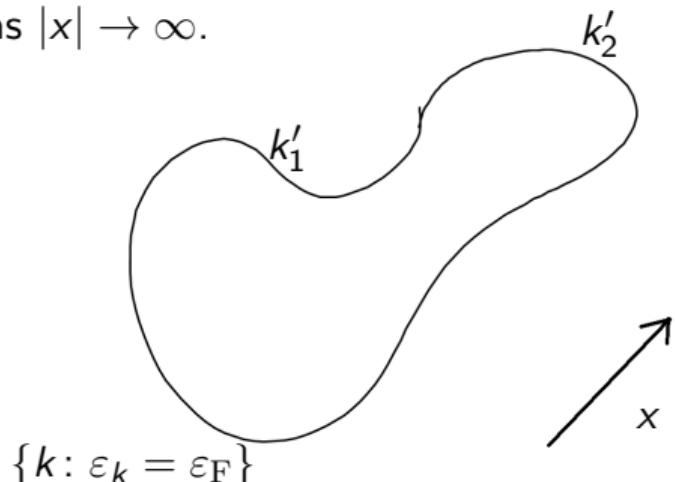
$$H \varphi_i = \lambda_i \varphi_i$$

Scattering Theory: Eigenfunction Expansions

- For $V \in L^p \cap L^{\frac{d}{d-1}}$, $\exists! \Psi_k^+$ with $|V|^{\frac{p}{2}} \Psi_k^+ \in L^2$ ($1 \leq p < \frac{d}{d-1}$)
- Asymptotics Green's function (see poster) \Rightarrow

$$\Psi_k^+(x) \approx \Psi_k(x) + \sum_{k'} c_{k'} \frac{e^{ik' \cdot x}}{|x|^{\frac{d-1}{2}}} \underbrace{\langle \Psi_{k'} | V | \Psi_k^+ \rangle}_{=: T(k', k)}$$

as $|x| \rightarrow \infty$.



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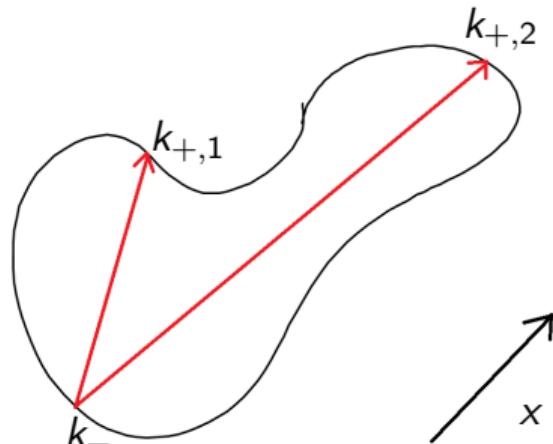
$$H = H_0 + V,$$
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$$H \varphi_i = \lambda_i \varphi_i$$

$$\Psi_k^+ := \Omega^+ \Psi_k$$
$$\Psi_k^+ = \Psi_k + G_0(\varepsilon_k) V \Psi_k^+$$

Scattering Theory: Eigenfunction Expansions

$$\begin{aligned}\rho_V(x) - \rho_0(x) &= \int_{\mathcal{B}} f_{\varepsilon_F}(\varepsilon_k) \left[|\Psi_k^+|^2 - |\Psi_k|^2 \right] dk = \dots = \\ &= C \frac{\text{Re}}{|x|^d} \sum_{k_-, k_+} c_{k_-} c_{k_+} \Psi_{k_+}(x) T(k_+, k_-) \overline{\Psi_{k_-}(x)}\end{aligned}$$

as $|x| \rightarrow \infty$.



more details

Notation:

$$\begin{aligned}H_0 &= -\Delta + W_{\text{per}}, \\ \Psi_k &= u_k(x) e^{ik \cdot x} \text{ with} \\ H_0 \Psi_k &= \varepsilon_k \Psi_k, \\ G_0(E) &:= (E + i0^+ - H_0)^{-1}\end{aligned}$$

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$$T(k', k) := \langle \Psi_{k'} | V | \Psi_k^+ \rangle$$



Summary

- Finite temperature, insulators, metals at zero temperature exhibit different screening behaviour
- Green's function \implies linear response properties (see poster)
- Scattering theory \implies decay of $\rho_V - \rho_0$

Next:

- fixed point arguments to solve $V = V_{\text{def}} + v_c(\rho_V - \rho_0)$
e.g.

$$V_{n+1} = V_n + \frac{-\Delta}{1 - \Delta} [V_{\text{def}} + v_c(\rho_{V_n} - \rho_0) - V_n]$$

- More general Fermi surfaces,
- e.g. Graphene,

Thank you for your attention!

Slides are online: jack.thomaslabs.co.uk/Herrsching

Ideas in the proof

$$\begin{aligned}
 \chi_0 V &= \oint_{\mathcal{C}} f_{\varepsilon_F}(z) R_z V R_z(x, x) \frac{dz}{2\pi i} \\
 &= \oint_{\mathcal{C}} f_{\varepsilon_F}(z) \int_{\mathcal{B}} R_z e^{iq \cdot x} V_q R_z(x, x) dq \frac{dz}{2\pi i} \\
 &= \oint_{\mathcal{C}} f_{\varepsilon_F}(z) \int_{\mathcal{B}} e^{iq \cdot x} [e^{-iq \cdot x} R_z e^{iq \cdot x}] V_q R_z(x, x) dq \frac{dz}{2\pi i} \\
 &= \int_{\mathcal{B}} e^{iq \cdot x} \left[\oint_{\mathcal{C}} f_{\varepsilon_F}(z) \int_{\mathcal{B}} R_{z,k+q} V_q R_{z,k}(x, x) dk \frac{dz}{2\pi i} \right] dq
 \end{aligned}$$

$$V = V_{\text{def}} + v_c(\rho_V - \rho_0)$$

Notation:

$$V = \int_{\mathcal{B}} V_q(x) e^{iq \cdot x} dq$$

$$AV = \int_{\mathcal{B}} (A_q V_q)(x) e^{iq \cdot x} dq$$

$$H_0 := -\Delta + W_{\text{per}}$$

$$H_{0,q} = \sum_n \varepsilon_{nq} |u_{nq}\rangle \langle u_{nq}|$$

$$\begin{aligned}
 \chi_{0,q} V &= \sum_{nm} \oint_{\mathcal{C}} \int_{\mathcal{B}} \frac{f_{\varepsilon_F}(z)}{(z - \varepsilon_{n,k+q})(z - \varepsilon_{mk})} |u_{n,k+q}\rangle \langle u_{n,k+q}| V |u_{mk}\rangle \langle u_{mk}|(x, x) dk \frac{dz}{2\pi i} \\
 &= \sum_{nm} \int_{\mathcal{B}} \frac{f_{\varepsilon_F}(\varepsilon_{n,k+q}) - f_{\varepsilon_F}(\varepsilon_{mk})}{\varepsilon_{n,k+q} - \varepsilon_{mk}} |u_{n,k+q}\rangle \langle u_{n,k+q}| V |u_{mk}\rangle \langle u_{mk}|(x, x) dk
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back



Scattering Theory: Eigenfunction Expansions

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Scattering Theory: Eigenfunction Expansions

$$\Omega^+ := \lim_{\eta \downarrow 0} \int_{-\infty}^0 \eta e^{\eta t} e^{iHt} e^{-iH_0 t} dt$$

$$\begin{aligned}\Psi_k^+ &= \lim_{\eta \downarrow 0} \int_{-\infty}^0 \eta e^{\eta t} e^{iHt} e^{-iH_0 t} \Psi_k dt \\ &= \lim_{\eta \downarrow 0} \eta \int_{-\infty}^0 e^{-i(\varepsilon_k + i\eta - H)t} \Psi_k dt \\ &= \lim_{\eta \downarrow 0} \frac{i\eta}{\varepsilon_k + i\eta - H} \Psi_k =: \lim_{\eta \downarrow 0} i\eta G(\varepsilon_k + i\eta) \Psi_k \\ &= \lim_{\eta \downarrow 0} i\eta \left[G_0(\varepsilon_k + i\eta) + G_0(\varepsilon_k + i\eta) V G(\varepsilon_k + i\eta) \right] \Psi_k \\ &= \Psi_k + G_0(\varepsilon_k + i0^+) V \Psi_k^+\end{aligned}$$

back

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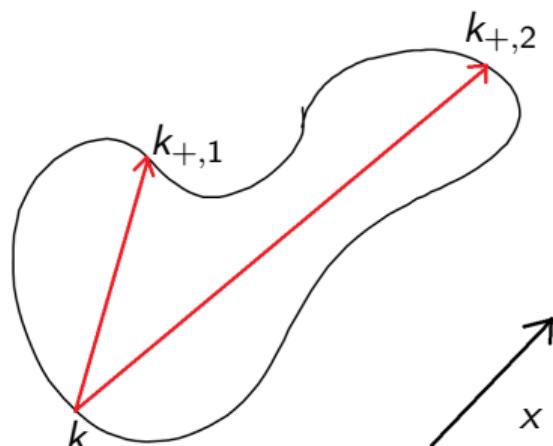
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Scattering Theory: Eigenfunction Expansions

Unitarity of T : if $\varepsilon_k = \varepsilon_{k'} = \varepsilon$, then

$$T(k, k') - \overline{T(k', k)} = \frac{2\pi i}{|\mathcal{B}|} \int_{\varepsilon_{k''}=\varepsilon} T(k, k'') T(k'', k') \frac{dk''}{|\nabla \varepsilon_{k''}|}$$



back

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