

Screening in the reduced Hartree–Fock model

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Mathematical Physics and PDEs
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Slides are online: jack.thomaslabs.co.uk/Herrsching

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

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

Vacuum

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

Coulomb potential

Total screening

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

Yukawa potential with screening length k^{-1}

Partial screening

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

Dielectric constant of the material $\epsilon_r > 1$

Reduced Hartree–Fock (rHF) - finite systems

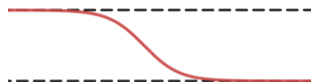
Coulomb operator:

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

Potential-to-density:

$$F_{\varepsilon_F}(V)(x) = f_{\varepsilon_F}(-\Delta + V)(x, x)$$
$$f_{\varepsilon_F}(x) = \left(1 + e^{\frac{x - \varepsilon_F}{k_B T}}\right)^{-1}$$

Fermi–Dirac distribution:



k_B - Boltzmann const.

T - temperature

ε_F - Fermi level

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

- 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

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

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

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:

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

Finite 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:

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

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

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

V_{ext} = external potential

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

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

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



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, $K = K' = 0$

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

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

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

Notation:

$$\begin{aligned} V &= \int_{\mathcal{B}} V_q(x) e^{iq \cdot x} dq \\ AV &= \int_{\mathcal{B}} (A_q V_q)(x) e^{iq \cdot x} dq \end{aligned}$$

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

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

[more details](#)



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

- 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

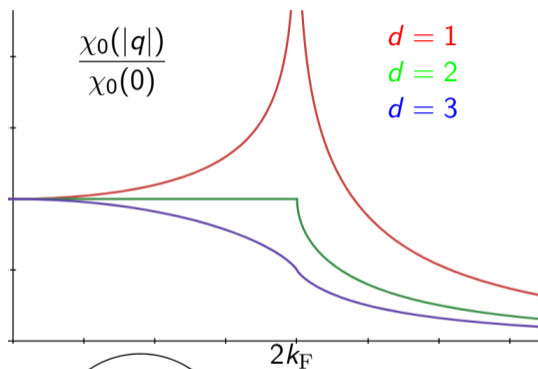
$$\chi_{0,00}(q) = \int_{\mathcal{B}} \frac{f_{\varepsilon_F}(\varepsilon_{k+q}) - f_{\varepsilon_F}(\varepsilon_k)}{\varepsilon_{k+q} - \varepsilon_k} |\langle u_k, u_{k+q} \rangle|^2 dk$$

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

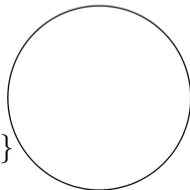
$$V(V_{\text{def}}) \approx \varepsilon^{-1} V_{\text{def}} = (1 - v_c \chi_0)^{-1} \frac{Q}{|x|}$$

$$\sim Q \frac{\sin(2k_F |x| + (d-2)\frac{\pi}{2})}{|x|^d}$$

as $|x| \rightarrow \infty$.



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



Metals at Zero Temperature

More generally,

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

where

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

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

QR

Friedel Oscillations
in the reduced Hartree-Fock model
Jack Thomsen, joint work with Antoine Leoni

Mathématiques
d'Orsay

Abstract: Friedel oscillations appear in a metal, the scattered electrons and the total potential being kept constant by the electron sea. In the homogeneous reduced Hartree-Fock model, still adding an exponentially screened $\delta(x)$, the total energy is stationary against exponentially screened perturbations. At any temperature, the position of the Fermi surface has to satisfy balance with the temperature given responsibility to be able to find a trace of Friedel oscillations for total potential surface and those approximately with respect to the dimension.

Suppose we have a lattice $\Lambda \subset \mathbb{Z}^d$ and an isolated well V , we let $\mathcal{C} := \mathbb{Z}^d \setminus \Lambda$. We consider for a fixed particle potential $H_{\mathcal{C}} := \mathcal{C}_{\mathcal{C}}^*$ associated Fermi level μ , consider the response to an effective potential V :

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

where $G_0(x, y; E) := \int_{\mathcal{B}} \frac{u_k(x) u_k^*(y)}{E + i\eta - \epsilon_k} e^{ik \cdot (x-y)} dk$ is the free Green's function with temperature $\eta > 0$ and \mathcal{B} is the Brillouin zone in \mathbb{R}^d .

Free temperature:

- $\chi_0 V$ decays "as waves of η ".
- $\chi_0 V$ oscillates with an amplitude that vanishes as $\eta \rightarrow 0$ along responsibility.

Zero temperature:

- A Fermi surface leads to fundamentally different behavior.
- $\chi_0 V$ oscillates and decays logarithmically with size depending on the Fermi surface.

Shape of the Fermi Surface

Now assuming response given in terms of the Green's function G_0 :

$$\chi_0 V(x) = \int_{\mathcal{B}} \int_{\mathcal{C}} G_0(x, y; E) V(y) G_0(y, x; E) dy dE$$

where $\chi_0 = \chi_0(x) = \chi_0(y) = \chi_0(z) = \dots$

$$-\chi_0 = \chi_0^2 = \chi_0^3 = \chi_0^4 = \dots = \chi_0^{\infty} = \chi_0^{\infty} = \chi_0^{\infty} = \dots$$

Therefore, the off-diagonal decay of χ_0 tells us corresponding rate of decay for χ_0 and χ_0^2, \dots

Proposition: As $\eta \rightarrow 0$, $\chi_0 V(x)$ behaves like $\chi_0 V(x) \sim \chi_0 V(x) + \chi_0^2 V(x) + \dots$ as $\eta \rightarrow 0$ (see [1]).

Proposition: The off-diagonal decay of χ_0 tells us corresponding rate of decay for χ_0 and χ_0^2, \dots

Theorem: A $\chi_0 V$ decays asymptotically as $\chi_0 V(x) \sim \chi_0 V(x) + \chi_0^2 V(x) + \dots$ as $\eta \rightarrow 0$ (see [1]).

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Figure 1: Diagram of a lattice with a central well V and Fermi surface \mathcal{F} . The Fermi surface is a sphere in \mathbb{R}^d . The Brillouin zone is a cube in \mathbb{R}^d . The Fermi surface is the intersection of the Brillouin zone and a sphere of radius k_F . The Fermi surface is a sphere in \mathbb{R}^d . The Brillouin zone is a cube in \mathbb{R}^d . The Fermi surface is the intersection of the Brillouin zone and a sphere of radius k_F .

Figure 2: Plots of Friedel oscillations for different Fermi surface shapes. The plots show the response $\chi_0 V(x)$ versus distance R . The left plot shows a smooth decay for a spherical Fermi surface. The middle plot shows oscillations for a square Fermi surface. The right plot shows oscillations for a hexagonal Fermi surface.

Figure 3: 3D visualization of Brillouin zones for different Fermi surfaces. The left plot shows a spherical Fermi surface. The middle plot shows a square Fermi surface. The right plot shows a hexagonal Fermi surface.

Scattering Theory: Eigenfunction Expansions

- Want: $\rho_V - \rho_0$,

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

$$\rho_V(x) \stackrel{?}{=} \sum_{j: \lambda_j \leq \varepsilon_F} |\varphi_j(x)|^2 + \int_B f_{\varepsilon_F}(\varepsilon_k) |\Psi_k^+(x)|^2 dk$$

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

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

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

- Lippmann-Schwinger: $\Psi_k^+ = \Psi_k + G_0(\varepsilon_k) V \Psi_k^+$

Proof

Notation:

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

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

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

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

$$H = H_0 + V,$$

$$G(E) := (E + i0^+ - H)^{-1}$$

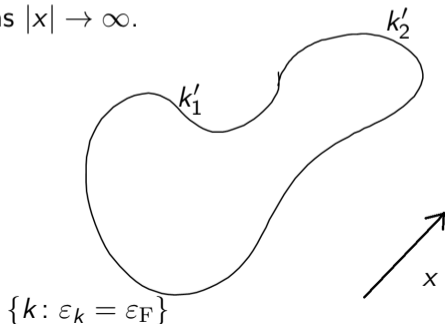
$$H \varphi_i = \lambda_i \varphi_i$$

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) \implies

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

as $|x| \rightarrow \infty$.



Notation:

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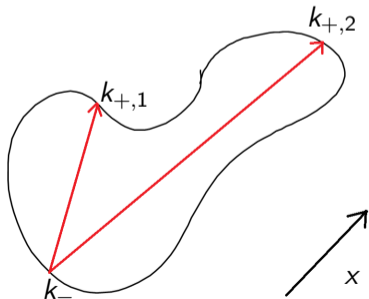
$$\Psi_k^+ := \Omega^+ \Psi_k$$

$$\Psi_k^+ = \Psi_k + G_0(\epsilon_k) V \Psi_k^+$$

Scattering Theory: Eigenfunction Expansions

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

as $|x| \rightarrow \infty$.



more details

Notation:

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$$\Psi_k^+ := \Omega^+ \Psi_k$$

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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

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

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

Notation:

$$V = \int_B V_q(x) e^{iq \cdot x} dq$$

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

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

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

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

[back](#)



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back

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



Scattering Theory: Eigenfunction Expansions

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

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

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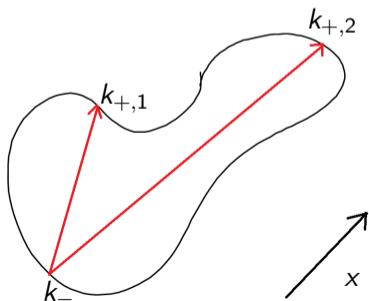
$$H\varphi_i = \lambda_i \varphi_i$$



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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