

Screening in the reduced Hartree–Fock model

Jack Thomas

Joint work with Antoine Levitt (Universite Paris–Saclay)
and Eric Cancès (Ecole des ponts ParisTech)

Mathematical Physics and PDEs
Herrsching, 16 December 2024,



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

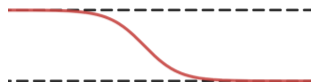
Coulomb operator:

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

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

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_{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:

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

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

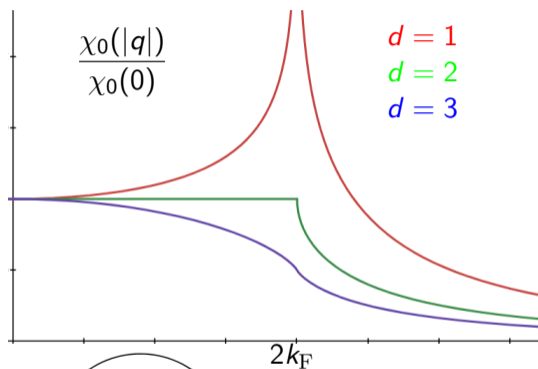
$$\chi_{0,00}(q) = \int_{\mathcal{B}} \frac{f_{\varepsilon_F}(\varepsilon_{k+q}) - f_{\varepsilon_F}(\varepsilon_k)}{\varepsilon_{k+q} - \varepsilon_k} |\langle u_k, u_{k+q} \rangle|^2 dk$$

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

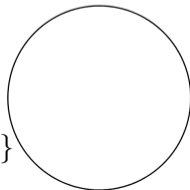
$$V(V_{\text{def}}) \approx \varepsilon^{-1} V_{\text{def}} = (1 - v_c \chi_0)^{-1} \frac{Q}{|x|}$$

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

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

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

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

Friedel Oscillations in the reduced Hartree-Fock model
 Jack Thoenes, joint work with Antoine Louch
 Département de Mathématiques d'Orsay

Abstract. Friedel oscillations around a central, neutral impurity and the total potential energy $\chi_0 V$ are derived for the electron. In the Fermi liquid reduced Hartree-Fock model, small deviations are considered around $\chi_0 V$, the total energy is obtained stationary, in the other hand, in the stationary phase approximation. The stationary phase approximation is used to study the asymptotic behaviour of the total energy $\chi_0 V$ in terms of the distance R of the Fermi surface $S(E)$ to the impurity V and the dimensionality of the system.

Introduction. In this paper we consider a central, neutral impurity and the total potential energy $\chi_0 V$ are derived for the electron. In the Fermi liquid reduced Hartree-Fock model, small deviations are considered around $\chi_0 V$, the total energy is obtained stationary, in the other hand, in the stationary phase approximation. The stationary phase approximation is used to study the asymptotic behaviour of the total energy $\chi_0 V$ in terms of the distance R of the Fermi surface $S(E)$ to the impurity V and the dimensionality of the system.

1.1. The Fermi liquid reduced Hartree-Fock model. The Fermi liquid reduced Hartree-Fock model is defined by the stationary Schrödinger equation $(-\Delta + V - \epsilon_F) \psi = 0$ in \mathbb{R}^d where ψ is the Fermi liquid wave function, V is the impurity potential, ϵ_F is the Fermi energy.

1.2. The total energy. The total energy E is given by $E = \int_{\mathbb{R}^d} |\nabla \psi|^2 dx + \int_{\mathbb{R}^d} V \psi^2 dx - \int_{\mathbb{R}^d} \psi^2 dx$.

1.3. The stationary phase approximation. The stationary phase approximation is used to study the asymptotic behaviour of the total energy $\chi_0 V$ in terms of the distance R of the Fermi surface $S(E)$ to the impurity V and the dimensionality of the system.

1.4. The asymptotic behaviour. The asymptotic behaviour of the total energy $\chi_0 V$ is given by $\chi_0 V \sim \frac{1}{R^{d-2}}$ as $R \rightarrow \infty$.

1.5. The Friedel oscillations. The Friedel oscillations are given by $\chi_0 V \sim \frac{1}{R^{d-2}} \cos(k_F R)$ as $R \rightarrow \infty$.




Figure 1. Decay of the Green's function $G_0(x, y; E)$ for three dimensions $d=1, 2, 3$. The plots show the magnitude of $G_0(x, y; E)$ versus the distance R . The curves exhibit oscillatory decay as R increases, with the amplitude decreasing as $R \rightarrow \infty$.

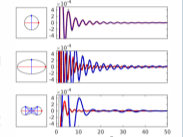


Figure 2. Decay of $\chi_0 V$ for the three most Fermi surface shapes. The plots show $\chi_0 V$ versus R for $d=1, 2, 3$. The curves show oscillatory decay with increasing R , and the amplitude decreases as $R \rightarrow \infty$.

1.6. The asymptotic behaviour of $\chi_0 V$. The asymptotic behaviour of $\chi_0 V$ is given by $\chi_0 V \sim \frac{1}{R^{d-2}}$ as $R \rightarrow \infty$.

1.7. The Friedel oscillations. The Friedel oscillations are given by $\chi_0 V \sim \frac{1}{R^{d-2}} \cos(k_F R)$ as $R \rightarrow \infty$.

1.8. The asymptotic behaviour of $\chi_0 V$ in terms of the distance R . The asymptotic behaviour of $\chi_0 V$ is given by $\chi_0 V \sim \frac{1}{R^{d-2}}$ as $R \rightarrow \infty$.

1.9. The asymptotic behaviour of $\chi_0 V$ in terms of the dimensionality of the system. The asymptotic behaviour of $\chi_0 V$ is given by $\chi_0 V \sim \frac{1}{R^{d-2}}$ as $R \rightarrow \infty$.

1.10. The asymptotic behaviour of $\chi_0 V$ in terms of the Fermi energy ϵ_F . The asymptotic behaviour of $\chi_0 V$ is given by $\chi_0 V \sim \frac{1}{R^{d-2}}$ as $R \rightarrow \infty$.

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:

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

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

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

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

$$H = H_0 + V,$$

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

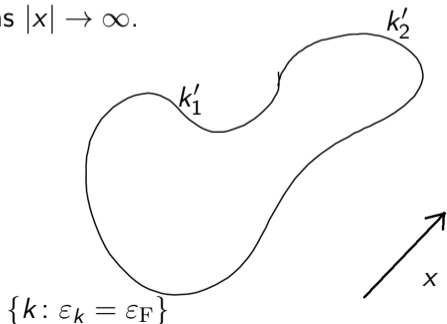
$$H \varphi_i = \lambda_i \varphi_i$$

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:

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

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

$$H_0 \Psi_k = \epsilon_k \Psi_k,$$

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

$$H = H_0 + V,$$

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

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

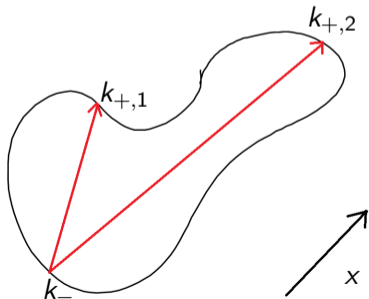
$$\Psi_k^+ := \Omega^+ \Psi_k$$

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

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:

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

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

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

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

$$H = H_0 + V,$$

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

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

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

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

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

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:

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

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

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

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

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

[back](#)



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

back

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

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

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

back

Notation:

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

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

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

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

$$H = H_0 + V,$$

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

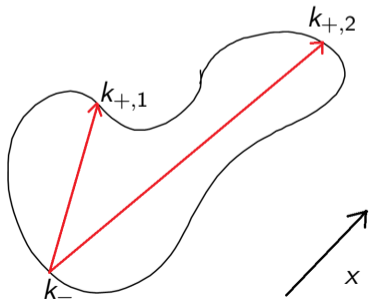
$$H\varphi_i = \lambda_i \varphi_i$$



Scattering Theory: Eigenfunction Expansions

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

Notation:

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

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

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

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

$$H = H_0 + V,$$

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

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

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

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

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

