Screening in the reduced Hartree–Fock model

Jack Thomas

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

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Slides are online: `jack.thomaslabs.co.uk/L'Aquila`

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1. Screening
2. reduced Hartree–Fock (rHF)
3. Screening in rHF (finite temperature & insulators)
4. (if time) Metals at $T = 0$

Outline

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Electrostatic Screening: $V_{\mathrm{def}}(x) = \frac{Q}{|x|}$

- Point charge in vacuum $\implies$ long-range Coulomb potential
- In a material $\implies$ material reorganises itself, total potential (Coulomb + response) is screened,

$$V_{\mathrm{tot}} \approx \epsilon^{-1} V_{\mathrm{def}}$$

- Behaviour depends on whether charge carriers are mobile,
- Empirical models:

Vacuum

$$V_{\mathrm{tot}}(x) = \frac{Q}{|x|},$$

Coulomb potential

Total screening

$$V_{\mathrm{tot}}(x) = \frac{Q}{|x|} e^{-k|x|}$$

Yukawa potential with screeening length k^{-1}

Partial screening

$$V_{\mathrm{tot}}(x) = \frac{Q}{\varepsilon_r |x|}$$

Dielectric constant of the material $\varepsilon_r > 1$

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reduced Hartree–Fock (rHF) - finite systems

Finite Systems

Total potential V_{tot} satisfies:

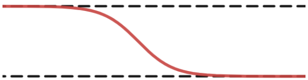
$$V_{\text{tot}} = V_{\text{ext}} + v_c F_{\varepsilon_F}(V_{\text{tot}})$$

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

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

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

Fermi–Dirac distribution:



Coulomb operator:

$$v_c \rho = |x|^{-1} \star \rho$$

Potential-to-density:

$$F_{\varepsilon_{\mathrm{F}}}(V) = \operatorname{den} f_{\varepsilon_{\mathrm{F}}}\left(-\Delta + V\right)$$

$$f_{\varepsilon_{\mathrm{F}}}(x) = \left(1 + e^{\frac{x-\varepsilon_{\mathrm{F}}}{k_{\mathrm{B}}T}}\right)^{-1}$$

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T - temperature
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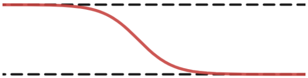

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reduced Hartree–Fock (rHF) - periodic problem

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

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]

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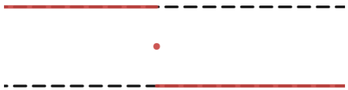

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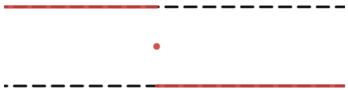

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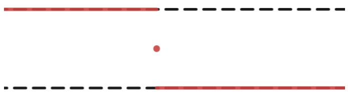

reduced Hartree–Fock (rHF) – defect problem

$$\Longrightarrow \quad W_{\mathrm{per}} = W_{\mathrm{nucl}} + v_{\mathrm{per}} F_{\varepsilon_{\mathrm{F}}}(W_{\mathrm{per}})$$

unique solution of the periodic rHF problem

Defect Problem

Change in total potential V due to defect potential V_{def}:

$$V = V_{\mathrm{def}} + v_c(\rho_V - \rho_0)$$
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Linearise:

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Screening in rHF: finite temperature & insulators

- $H_0 := -\Delta + W_{\mathrm{per}}$, $H_{0,q} = \sum_n \varepsilon_{nq} \left|u_{nq}\right\rangle \left\langle u_{nq}\right|$
- Look at $\chi_0 = F'_{\varepsilon_{\mathrm{F}}}(W_{\mathrm{per}})$: Use

$$F_{\epsilon_{\mathrm{F}}}(W_{\mathrm{per}} + V) = \oint_{\mathscr{C}} f_{\epsilon_{\mathrm{F}}}(z)\,(z - H_0 - V)^{-1}\,\frac{\mathrm{d}z}{2\pi i}$$

to obtain

$$\begin{aligned}\langle W_1, \chi_{0,q} W_2\rangle &= \sum_{nm} \fint_{\mathcal{B}} \frac{f_{\epsilon_{\mathrm{F}}}(\varepsilon_{n,k+q}) - f_{\epsilon_{\mathrm{F}}}(\varepsilon_{mk})}{\varepsilon_{n,k+q} - \varepsilon_{mk}} \langle W_1 u_{mk}, u_{n,k+q}\rangle \langle u_{n,k+q}, W_2 u_{mk}\rangle\,\mathrm{d}k \\ &\approx \sum_n \fint_{\mathcal{B}} f'_{\varepsilon_{\mathrm{F}}}(\varepsilon_{nk})|u_{nk}|^2 \mathrm{d}k + \sum_{n\neq m} \fint_{\mathcal{B}} \frac{f_{\varepsilon_{\mathrm{F}}}(\varepsilon_{nk}) - f_{\varepsilon_{\mathrm{F}}}(\varepsilon_{mk})}{(\varepsilon_{n,k} - \varepsilon_{mk})^3} |\langle q\cdot\nabla u_{mk}, u_{nk}\rangle|^2\,\mathrm{d}k \\ &= -\mathrm{DOS} - q^T L q\end{aligned}$$

where $\mathrm{DOS} \geq 0$ and $0 \leq L \in \mathbb{R}^3_{\mathrm{sym}}$.

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Notation:
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$$\approx \sum_{n} ⨍_{\mathcal{B}} f'_{\varepsilon_{\mathrm{F}}}(\varepsilon_{nk}) |u_{nk}|^2 \mathrm{d}k + \sum_{n\neq m} ⨍_{\mathcal{B}} \frac{f_{\varepsilon_{\mathrm{F}}}(\varepsilon_{nk}) - f_{\varepsilon_{\mathrm{F}}}(\varepsilon_{mk})}{(\varepsilon_{n,k} - \varepsilon_{mk})^3} \left|\langle q\cdot\nabla u_{mk}, u_{nk}\rangle\right|^2 \mathrm{d}k$$

$$= -\mathrm{DOS} - q^T L q$$

where $\mathrm{DOS} \geq 0$ and $0 \leq L \in \mathbb{R}^3_{\mathrm{sym}}$.

more details

Screening in rHF: finite temperature & insulators

- $H_0 := -\Delta + W_{\mathrm{per}}$, $H_{0,q} = \sum_n \varepsilon_{nq} \left| u_{nq} \right\rangle \left\langle u_{nq} \right|$
- Look at $\chi_0 = F'_{\varepsilon_{\mathrm{F}}}(W_{\mathrm{per}})$: Use

$$F_{\epsilon_{\mathrm{F}}}(W_{\mathrm{per}} + V) = \oint_{\mathscr{C}} f_{\epsilon_{\mathrm{F}}}(z)\,(z - H_0 - V)^{-1}\,\frac{\mathrm{d}z}{2\pi i}$$

to obtain

$$\langle W_1, \chi_{0,q} W_2 \rangle = \sum_{nm} \fint_{\mathcal{B}} \frac{f_{\epsilon_{\mathrm{F}}}(\varepsilon_{n,k+q}) - f_{\epsilon_{\mathrm{F}}}(\varepsilon_{mk})}{\varepsilon_{n,k+q} - \varepsilon_{mk}} \langle W_1 u_{mk}, u_{n,k+q} \rangle \langle u_{n,k+q}, W_2 u_{mk} \rangle \,\mathrm{d}k$$

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$$V = V_{\mathrm{def}} + v_c(\rho_V - \rho_0)$$
$$\approx (1 - v_{\mathrm{c}}\chi_0)^{-1} V_{\mathrm{def}}$$

Notation:

$V = \fint_{\mathcal{B}} V_q(x) e^{iq\cdot x} \mathrm{d}q$

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

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

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

  small defects are totally screened [A. Levitt, 2020]

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Application: Interatomic Force Constants, smeared nuclei

C_{IJ} := derivative of the force on atom I with respect to the postion of atom J:

$$\nu_{\mathrm{nucl}} = \sum_I Z_I m(\cdot - R_I), \qquad C_{IJ} = \frac{\partial F_I}{\partial R_J} = Z_I Z_J \left\langle \nabla m(\cdot - R_I), \epsilon^{-1} v_{\mathrm{c}} \nabla m(\cdot - R_J) \right\rangle$$

Theorem (E. Cancès, A. Levitt, JT, '25)

At finite temperature $T > 0$:

$$|C_{IJ}| \leq C e^{-\eta |R_I - R_J|}$$

with $\eta \geq c \min\{1, T\}$.

Theorem (E. Cancès, A. Levitt, JT, '25)

For insulators with $T = 0$,

$$C_{IJ} = (Z_I^\star)^T \nabla^2 \Phi_{M^{-1}}(R_I - R_J) Z_J^\star + \mathcal{O}(|R_I - R_J|^{-4})$$

where $Z^\star \in \mathbb{R}^{3\times 3}$ are *Born effective charges*, $\Phi_{M^{-1}}(x) := \frac{1}{\sqrt{\det M}} \frac{1}{\sqrt{x^T M^{-1} x}}$ is the *screened Coulomb operator*, and $M \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ is the *macroscopic dielectric permittivity*, $M \geq 1$.

On arXiv "soon"

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Outline

1. Screening
2. reduced Hartree–Fock (rHF)
3. Screening in rHF (finite temperature & insulators)
4. (if time) Metals at $T = 0$

Metals at $T = 0$: Free electron gas

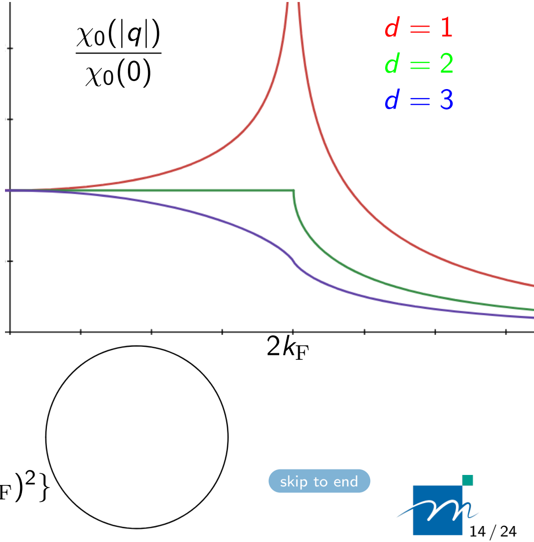
$$\chi_0(q) = \fint_{\mathcal{B}} \frac{f_{\varepsilon_\mathrm{F}}(\varepsilon_{k+q}) - f_{\varepsilon_\mathrm{F}}(\varepsilon_k)}{\varepsilon_{k+q} - \varepsilon_k} \left|\langle u_k, u_{k+q}\rangle\right|^2 \mathrm{d}k$$

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

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

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

as $|x| \to \infty$.



Friedel oscillations

$$\{k : \varepsilon_k = \varepsilon_\mathrm{F} =: (k_\mathrm{F})^2\}$$

skip to end

Scattering Theory: Eigenfunction Expansions

- Want: $\rho_V - \rho_0$,

$$\rho_0(x) = f_{\varepsilon_{\mathrm{F}}}(H_0)(x,x) = \int_{\mathcal{B}} f_{\varepsilon_{\mathrm{F}}}(\varepsilon_k)|\Psi_k(x)|^2 \mathrm{d}k$$

$$\rho_V(x) \overset{?}{=} \sum_{j:\,\lambda_j \le \varepsilon_{\mathrm{F}}} |\varphi_i(x)|^2 + \int_{\mathcal{B}} f_{\varepsilon_{\mathrm{F}}}(\varepsilon_k)|\Psi_k^+(x)|^2 \mathrm{d}k$$

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

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

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Notation:
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Scattering Theory: Eigenfunction Expansions

- For $V \in L^p \cap L^{\frac{d}{d-1}}$, $\exists! \Psi_k^+$ with $|V|^{\frac{p}{2}} \Psi_k^+ \in L^2 \quad (1 \leq p < \frac{d}{d-1})$

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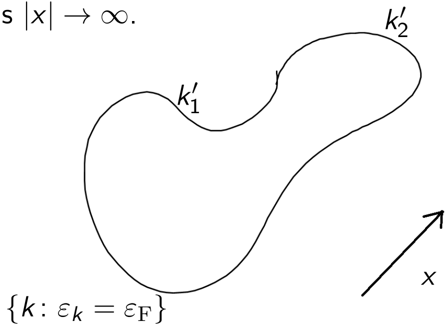
- Asymptotics Green's function $\implies$

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

as $|x| \to \infty$.



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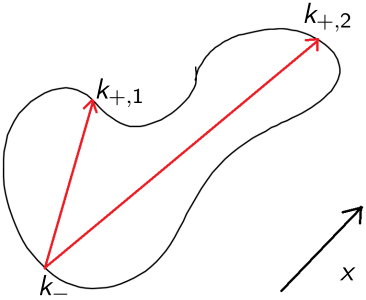
$$\rho_V(x) - \rho_0(x) = \fint_{\mathcal{B}} f_{\varepsilon_{\mathrm{F}}}(\varepsilon_k)\left[\left|\Psi_k^+\right|^2 - \left|\Psi_k\right|^2\right] \mathrm{d}k \quad = \cdots =$$

$$= C\frac{\mathrm{Re}}{|x|^d}\sum_{k_-,k_+} c_{k_-} c_{k_+} \Psi_{k_+}(x) T(k_+, k_-) \overline{\Psi_{k_-}(x)}$$

as $|x| \to \infty$.



more details

Notation:

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

$H = H_0 + V$,
$G(E) := (E + i0^+ - H)^{-1}$
$H\varphi_i = \lambda_i\varphi_i$

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

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

Summary

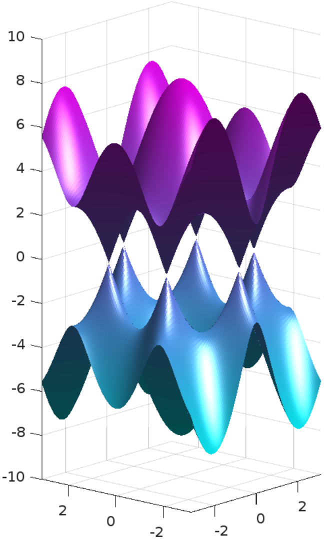
- Finite temperature, insulators, metals at zero temperature exhibit different screening behaviour
- Scattering theory $\implies$ decay of $\rho_V - \rho_0$

Next:

- fixed point arguments to solve $V = V_{\mathrm{def}} + v_c(\rho_V - \rho_0)$,
- More general Fermi surfaces,
  `https://www.phys.ufl.edu/fermisurface/`
- e.g. Graphene, ...

Thank you for your attention!

Slides are online: `jack.thomaslabs.co.uk/L'Aquila`



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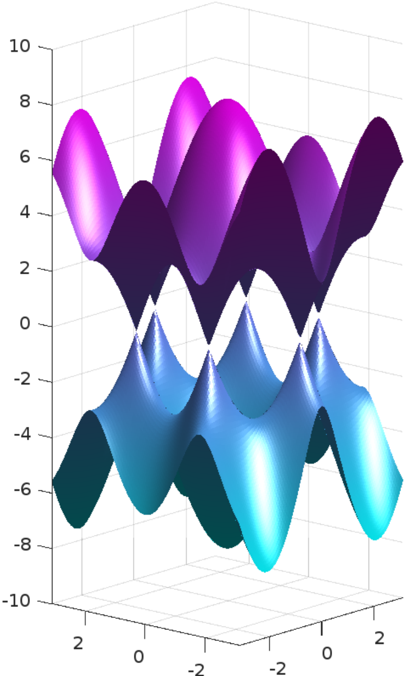
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6
4
2
0
-2
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-6
-8
-10
2
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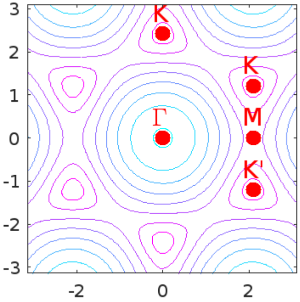
2


K
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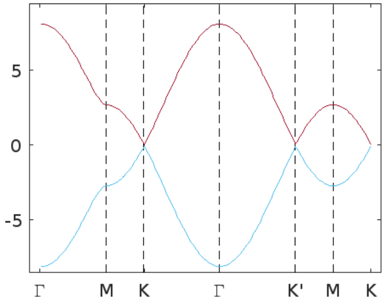
5
0
-5
Γ
M
K
Γ
K'
M
K

Ideas in the proof

$$
\begin{aligned}
\chi_0 V &= \oint_{\mathscr{C}} f_{\varepsilon_{\mathrm{F}}}(z)\ R_z V R_z(x,x)\ \frac{\mathrm{d}z}{2\pi i} \\
&= \oint_{\mathscr{C}} f_{\varepsilon_{\mathrm{F}}}(z)\ \fint_{\mathcal{B}} R_z e^{iq\cdot x} V_q R_z(x,x)\mathrm{d}q\ \frac{\mathrm{d}z}{2\pi i} \\
&= \oint_{\mathscr{C}} f_{\varepsilon_{\mathrm{F}}}(z)\ \fint_{\mathcal{B}} e^{iq\cdot x}\left[e^{-iq\cdot x} R_z e^{iq\cdot x}\right] V_q R_z(x,x)\mathrm{d}q\ \frac{\mathrm{d}z}{2\pi i} \\
&= \fint_{\mathcal{B}} e^{iq\cdot x}\left[\oint_{\mathscr{C}} f_{\varepsilon_{\mathrm{F}}}(z)\ \fint_{\mathcal{B}} R_{z,k+q} V_q R_{z,k}(x,x)\mathrm{d}k\ \frac{\mathrm{d}z}{2\pi i}\right]\mathrm{d}q
\end{aligned}
$$

$$V = V_{\mathrm{def}} + v_c\left(\rho_V - \rho_0\right)$$

Notation:

$$V = \fint_{\mathcal{B}} V_q(x) e^{iq\cdot x}\mathrm{d}q$$

$$AV = \fint_{\mathcal{B}}(A_q V_q)(x) e^{iq\cdot x}\mathrm{d}q$$

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

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

$$
\begin{aligned}
\chi_{0,q} V &= \sum_{nm} \oint_{\mathscr{C}} \fint_{\mathcal{B}} \frac{f_{\varepsilon_{\mathrm{F}}}(z)}{(z-\varepsilon_{n,k+q})(z-\varepsilon_{mk})}\ \left|u_{n,k+q}\right\rangle \left\langle u_{n,k+q}\right| V \left|u_{mk}\right\rangle \left\langle u_{mk}\right| (x,x)\mathrm{d}k\ \frac{\mathrm{d}z}{2\pi i} \\
&= \sum_{nm} \fint_{\mathcal{B}} \frac{f_{\varepsilon_{\mathrm{F}}}(\varepsilon_{n,k+q}) - f_{\varepsilon_{\mathrm{F}}}(\varepsilon_{mk})}{\varepsilon_{n,k+q} - \varepsilon_{mk}}\ \left|u_{n,k+q}\right\rangle \left\langle u_{n,k+q}\right| V \left|u_{mk}\right\rangle \left\langle u_{mk}\right| (x,x)\mathrm{d}k
\end{aligned}
$$

back

Scattering Theory: Eigenfunction Expansions

- Want: $\rho_V - \rho_0$,

$$\rho_0(x) = f_{\varepsilon_{\mathrm{F}}}(H_0)(x,x) = \fint_{\mathcal{B}} f_{\varepsilon_{\mathrm{F}}}(\varepsilon_k)|\Psi_k(x)|^2 \mathrm{d}k$$

$$\rho_V(x) \overset{?}{=} \sum_{j\colon \lambda_j \le \varepsilon_{\mathrm{F}}} |\varphi_i(x)|^2 + \fint_{\mathcal{B}} f_{\varepsilon_{\mathrm{F}}}(\varepsilon_k)|\Psi_k^+(x)|^2 \mathrm{d}k$$

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

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

- " $\Omega^+ = \lim_{t\to-\infty} e^{iHt} e^{-iH_0 t}$ ", $\quad \Omega^+ H = H_0 \Omega^+$
- Lippmann-Schwinger: $\Psi_k^+ = \Psi_k + G_0(\varepsilon_k) V \Psi_k^+$ back

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Scattering Theory: Eigenfunction Expansions

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

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

back

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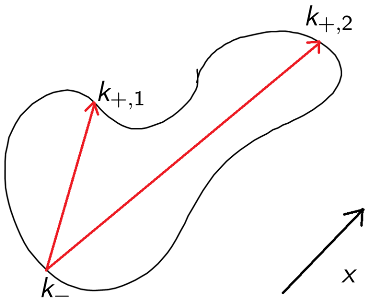
Scattering Theory: Eigenfunction Expansions

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

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



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