Friedel Oscillations
in the reduced Hartree–Fock model

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Abstract: When a defect potential is placed in a material, the material rearranges and the total potential at long-range is screened by the electrons. In the finite temperature reduced Hartree–Fock model, small defects are completely screened [3]; the total change in potential decays exponentially. On the other hand, in metals at zero temperature, the presence of the Fermi-surface introduces non-analytic behaviour into the independent-particle susceptibility χ_0, leading to what are known as Friedel oscillations; the total potential oscillates and decays algebraically, with exponent depending on the dimensionality and properties of the Fermi surface.

Introduction

Suppose we have a lattice $\mathbb{L} \subset \mathbb{R}^d$ and an associated unit cell Ω, we let $L^2_{\rm per} := \{f \in L^2(\Omega) \colon f \text{ is } \mathbb{L}\text{-periodic}\}$. For a fixed periodic potential $W_{\rm per} \in L^2_{\rm per}$ and Fermi level $\varepsilon_{\rm F}$, consider the response to an effective potential V:

$$\begin{aligned}\rho_V(x) &= F_{\varepsilon_{\rm F}}\big(-\Delta + W_{\rm per} + V\big)(x,x) \\ &= \rho_0(x) + \chi_0 V(x) + \cdots \end{aligned} \tag{1}$$

where
- $F_{\varepsilon_{\rm F}}(x) := \big(1 + e^{\frac{x-\varepsilon_{\rm F}}{k_{\rm B}T}}\big)^{-1}$ is the Fermi–Dirac distribution with temperature $T \geq 0$ and
- χ_0 is the independent particle susceptibility operator.

$$\begin{aligned} &\text{Linear model:} && V = V_{\rm def}, \\ &\text{Reduced Hartree–Fock (rHF):} && V = V_{\rm def} + \big(\rho_V - \rho_0\big) \star |\cdot|^{-1}, \end{aligned} \tag{2}$$

Finite temperature:
- $\chi_0 V$ decays "as quickly as" V,
- rHF: small defects are completely screened; $V(V_{\rm def})$ in (2) decays exponentially [3].

Zero temperature:
- Fermi surface leads to fundamentally different behaviour,
- $\rho_V - \rho_0$ oscillates and decays algebraically with rate depending on the Fermi surface,
- **Aim:** For small $V_{\rm def}$, solve (2) in weighted Sobolev spaces.

Notation: $\mathbb{L}^\star$ reciprocal lattice with unit cell $\Omega^\star$,
$H_0 := -\Delta + W_{\rm per}$ has eigenpairs: ε_{nk}, $\Psi_{nk}(x) = u_{nk}(x)e^{ik\cdot x}$ for $k \in \Omega^\star$, [u_{nk} is $\mathbb{L}$-periodic]
$S(E) = \bigcup_n S_n(E)$, $S_n(E) := \{k \in \Omega^\star \colon \varepsilon_{nk} = E\}$. [$S(\varepsilon_{\rm F})$ = Fermi surface]

Decay of the Green's Function

Non-interacting response given in terms of the Green's function G^E_V:

$$\rho_V(x) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_{\rm F}} G^E_V(x,x)\,\mathrm{d}E \tag{3}$$

where

$$\begin{aligned} G^E_V &:= \lim_{\eta\downarrow 0}\big(E - H_0 - V + i\eta\big)^{-1} && \big[H_0 := -\Delta + W_{\rm per}\big] \\ &= G^E_0 + G^E_0 V G^E_0 + G^E_0 V G^E_0 V G^E_0 + G^E_0 V G^E_0 V G^E_0 V G^E_0 + \cdots && [\text{Dyson series}] \\ &=: G^E_0 + G^E_0 T^E G^E_0 && \big[T^E := V(1 - G^E_0 V)^{-1} = \text{transfer matrix}\big] \end{aligned}$$

If V decays at infinity, $E \mapsto T^E$ is "smooth" and "localising"
[for $V \in L^2_{2s}$, we have $E \mapsto T^E$ is of class $C^{s-\frac12}\big(\mathbb{R}\setminus\mathscr{E}; \mathcal{L}(H^2_{-s}, L^2_s)\big)$
where $H^k_s := \{f \colon (1+|x|^2)^{\frac{s}{2}} f \in H^k\}$ and $\mathscr{E}$ is closed and discrete]

Proposition 1: Decay of the Green's function. Suppose that $S(E)$ has non-zero Gauss curvature at all points $k \in S(E)$ with normal in the direction $x - y$. Then,

$$G^E_0(x,y) = R^{-\frac{d-1}{2}} \sum_{\substack{k \in S_n(E)\colon \\ \frac{\nabla\varepsilon_{nk}}{|\nabla\varepsilon_{nk}|} = \frac{x-y}{|x-y|}}} c_k \Psi_{nk}(x)\overline{\Psi_{nk}(y)} + O\big(R^{-\frac{d+1}{2}}\big) \tag{4}$$

as $R := |x-y| \to \infty$, where $c_k := \frac{C_d}{|\nabla\varepsilon_{nk}|}\frac{e^{-i\frac{\pi}{4}\sum_{j=1}^{d-1}\mathrm{sgn}\,\kappa_{kj}}}{\prod_{j=1}^{d-1}\sqrt{|\kappa_{kj}|}}$ and $\{\kappa_{kj}\}$ are the principal curvatures of $S(E)$ at k.

Ideas of the Proof. Write G^E_0 in Fourier and apply co-area formula to replace $\int_{\Omega^\star}$ with $\int_{\mathbb{R}}\int_{S(\varepsilon)}\frac{1}{|\nabla\varepsilon_{nk}|}$. Use Plemelj formula: $\frac{1}{\varepsilon - i0^+} = \mathrm{p.v.}\,\frac{1}{\varepsilon} + \mathrm{i}\pi\delta = \sqrt{2\pi}\mathrm{i}\widehat{\mathbf{1}_{\mathbb{R}_+}}(\varepsilon)$ and conclude by stationary phase arguments on $\int_{S(E)}$. □

Remark: For $d = 2$, we may rotate so that $\frac{x-y}{|x-y|} = \binom{0}{1}$ and near $k \in S(E)$ with $\frac{\nabla\varepsilon_{nk}}{|\nabla\varepsilon_{nk}|} = \frac{x-y}{|x-y|}$, the surface is $\big\{k + \binom{\xi}{\phi(\xi,E)}\big\}$. Then the asymptotics of $G^E_0(x,y)$ can be written as (4) but with a different constant c_k and $\frac{d-1}{2}$ replaced with ℓ^{-1} where $\ell = \min\big\{\ell \colon \frac{\partial^\ell}{\partial\xi^\ell}\phi(0,E) \neq 0\big\}$.

Remark: For $d = 3$, if $S(E)$ has κ non-zero principal curvatures, we have $|G^E_0(x,y)| \lesssim R^{-\frac{\kappa}{2}}$. In general, the exact asymptotic behaviour depends on the Newton diagram of $\phi(\cdot, E)$ and is more complicated: e.g. [2].

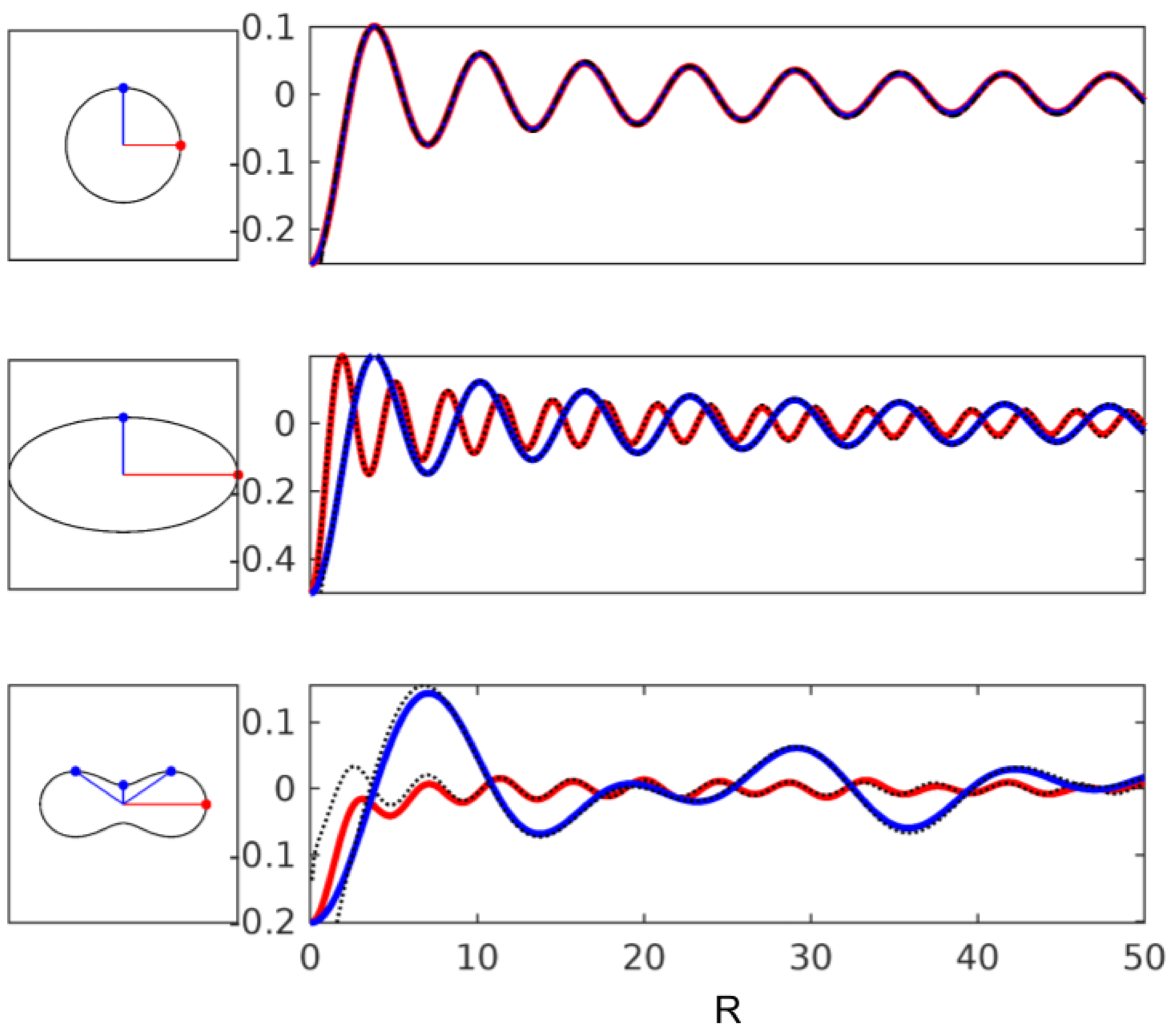

Figure 1: Decay of the Green's function for model Fermi surfaces in 2*d*.
Left: plots of the Fermi surface, together with points k in (4) for $x - y = R\binom{1}{0}$ (red) and $R\binom{0}{1}$ (blue).
Right: $\mathrm{Im}\,G^E_0(x,y)$ and the asymptotics from Proposition 1 (dotted) for $x - y = R\binom{1}{0}$ (red) and $R\binom{0}{1}$ (blue).

Non-interacting Response $\rho_V - \rho_0$

Proposition 2. Suppose that V has sufficient decay at infinity and $S(E)$ has non-zero Gauss curvature at all points $k \in S(E)$ with normal in the directions $\pm x$. Then,

$$\rho_V(x) - \rho_0(x) = |x|^{-d}\,\mathrm{Im}\sum_{\substack{k_+,k_- \in S(\varepsilon_{\rm F})\colon \\ \frac{\nabla\varepsilon_{k_\pm}}{|\nabla\varepsilon_{k_\pm}|} = \pm\frac{x}{|x|}}} c_{k_+k_-} u_{k_+}(x)\big\langle\Psi_{k_+}\big|T^{\varepsilon_{\rm F}}\big|\Psi_{k_-}\big\rangle\overline{u_{k_-}}(x)e^{i(k_+-k_-)\cdot x} + O(|x|^{-(d+1)}) \tag{5}$$

as $|x| \to \infty$, where $c_{k_+k_-} := \frac{i}{\pi}\frac{|\nabla\varepsilon_{k_+}||\nabla\varepsilon_{k_-}|}{|\nabla\varepsilon_{k_+}|+|\nabla\varepsilon_{k_-}|}c_{k_+}c_{k_-}$ and c_k is the constant from Proposition 1.

Remark: In the same spirit to the remarks following Proposition 1, one obtains a slower rate of decay when the Fermi surface is flatter at points $k_\pm$ in the summation in (5).

Remark: By a similar (but simpler) argument, we obtain the asymptotics for the independent particle susceptibility $\chi_0(x,y) \sim |x-y|^{-d}$. For simplicity, we plot $\chi_0(x,y)$ in Figure 2 instead of $\rho_V - \rho_0$.

Ideas of the Proof. For simplicity of notation, we consider $\chi_0(x,y)$ and set $u_{nk} \equiv 1$: by Proposition 1,

$$\chi_0(x,y) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_{\rm F}} G^E_0(x,y)G^E_0(y,x)\,\mathrm{d}E \sim |x-y|^{-(d-1)}\int_{-\infty}^{\varepsilon_{\rm F}}\sum_{k_+,k_-} c_{k_+}c_{k_-}e^{i(k_+-k_-)\cdot(x-y)}\,\mathrm{d}E \tag{6}$$

where $E \mapsto k_\pm(E) \in S(E)$ are smooth with $\frac{\nabla\varepsilon_{k_\pm}}{|\nabla\varepsilon_{k_\pm}|}\cdot\frac{x-y}{|x-y|} = \pm 1$. Moreover,
$\frac{\mathrm{d}}{\mathrm{d}E}\big(\pm k_\pm\cdot(x-y)\big)\big) = |\nabla\varepsilon_{k_\pm}|^{-1}|x-y|$. Therefore, one concludes by integration by parts. □

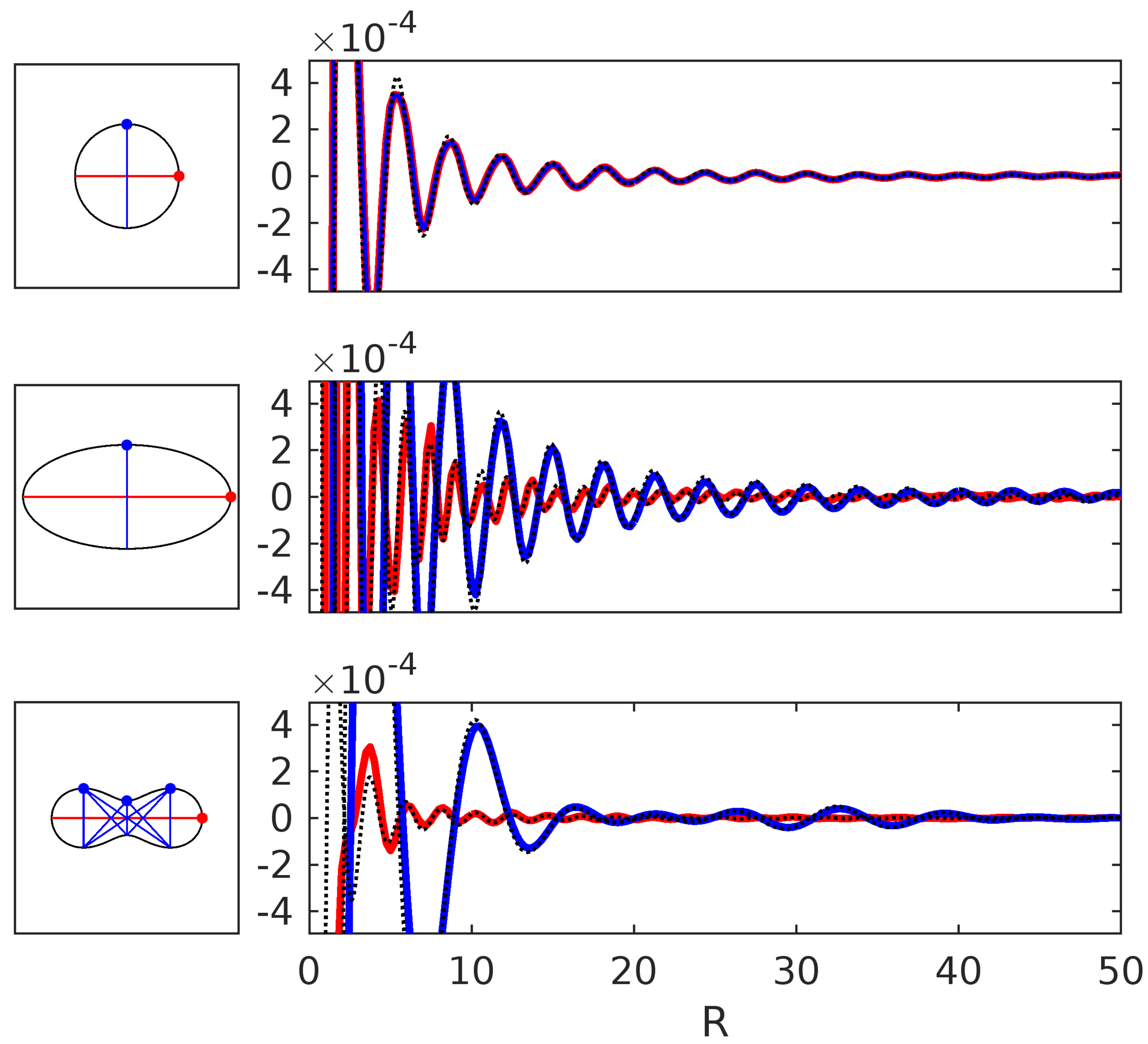

Figure 2: Decay of the linear response $\chi_0(x,y)$ for the model Fermi surfaces in Figure 1.
Left: plots of the Fermi surface, together with $k_+ - k_-$ as in (5) for $x - y = R\binom{1}{0}$ (red) and $R\binom{0}{1}$ (blue).
Right: $\chi_0(x,y)$ and the asymptotics that results from Prop. 1 (dotted) for $x - y = R\binom{1}{0}$ (red) and $R\binom{0}{1}$ (blue).

Conclusions & Remarks

- At finite temperature, $\rho_V - \rho_0$ decays as quickly as V, and $\rho_V - \rho_0 - \chi_0 V$ decays faster than V. This is a key fact that allows one to apply a fixed point argument to (2).
- At zero temperature, the situation is very different: we have shown that the response to an effective potential decays at most algebraically with rate depending on the dimension and Fermi surface,
- We have been unable thus far to extend the analysis to solve the fixed point problem (2).
- Under the same assumptions as Proposition 1, the density matrix $\rho_0(x,y)$ satisfies
$$\rho_0(x,y) = |x-y|^{-\frac{d+1}{2}}\,\mathrm{Im}\sum_k \widetilde{c}_k e^{ik\cdot(x-y)} + O\big(|x-y|^{-\frac{d+3}{2}}\big)$$
as $|x-y| \to \infty$, where the summation is over the same set as in (4) and $\widetilde{c}_k := \frac{i}{\pi}|\nabla\varepsilon_k|c_k$.
- Free electron gas: the decay of χ_0 results from the non-analytic behaviour of the Lindhard function [4, 5].

Future: Systems with degenerate Fermi surfaces (e.g. Graphene) and Fermi surfaces with vanishing curvature:

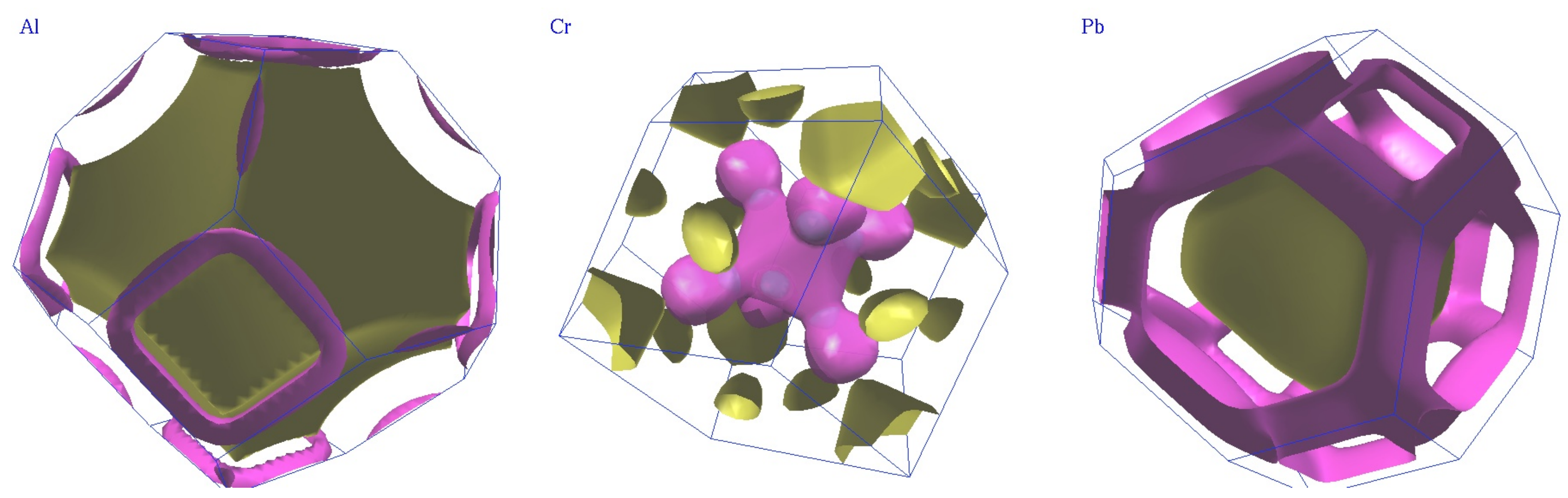

Figure 3: Examples of non-spherical Fermi surfaces. Left: Aluminium, Middle: Chromium, Right: Lead
Images taken from the Periodic Table of the Fermi Surfaces of Elemental Solids [1].

References

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[4] Bogdan Mihaila. *Lindhard function of a d-dimensional Fermi gas.* 2011. eprint: arXiv:1111.5337.

[5] George E. Simion and Gabriele F. Giuliani. "Friedel oscillations in a Fermi liquid". In: *Phys. Rev. B* 72.4 (2005).

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