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Decay of IFCs in rHF
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Why? Interatomic potentials & QM/MM methods

"$E(\underline{R}) \approx E(\underline{R}_0) + \frac{1}{2}(\underline{R}-\underline{R}_0)^T C (\underline{R}-\underline{R}_0)$"

"Interatomic Forces"

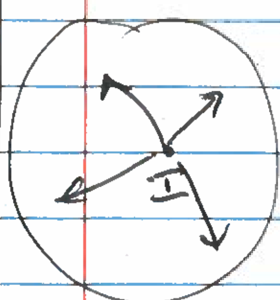
require → Force locality

Previously....

$|C_{IJ}| = \left|\frac{\partial F_I}{\partial R_J}\right| \to 0$ "sufficiently quickly" as $R_{IJ} \to \infty$

Energy locality in (linear) tight binding models

Recall, $E_I = [H f(H)]_{II}$ "site energy"



$$\left|\frac{\partial E_I}{\partial R_J}\right| \lesssim e^{-\eta_1 R_{IJ}}$$

$$\left|\frac{\partial^2 E_I}{\partial R_J \partial R_K}\right| \lesssim e^{-\eta_2 [R_{JI} + R_{IK}]}$$

$E = \sum_I E_I$ "Band energy"

$F_I = \frac{\partial E}{\partial R_I}$ "Force on atom I"

$C_{IJ} = \frac{\partial F_I}{\partial R_J}$ "IFC"

$$|C_{IJ}| \leq \sum_K \left|\frac{\partial^2 E_K}{\partial R_I \partial R_J}\right| \lesssim e^{-\frac{\eta_2}{2} r_{IJ}}$$

In TB models

Energy locality $\Longrightarrow$ locality of forces

__Want__ to include long-range Coulomb interactions

(R_I, Z_I) R_{IJ}^{-3} electrostatic potential

I

Ignore electrons:

moving atom J creates electrostatic potential R_{IJ}^{-3} at atom I

(R_J, Z_J)

J

d Charge dipole $Z_J d$

Including electrons

(1) finite temperature

* electrons are mobile
* "flock" towards the defect to screen the interaction at long-range

⇝ exponentially decaying force

(1) [Levitt 2020]

(2) [Cances, Deleurence, Lewin 2008]

[Cances, Lewin 2010]

Paper prove this for rHF

Proof Analyse regularity of the Fourier dual

"Dynamical Matrix"

(2) Insulator at zero temp

* electrons tightly bound to nuclei
* move rigidly w/ nuclei
* decreases eff. charge
* polarise

⇝ effective dielectric constant > vacuum

Partial screening

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$\boxed{\text{rHF} \atop \text{for a finite system}}$ — HF w/o exchange
— "Random phase approximation"

* N_{el} electrons
* nuclear distribution $\rho^{nuc}(x) = \sum_{k=1}^{K} Z_k m_k(x - R_k)$
probability measure

$1 = \hbar = m = e$
$\frac{1}{4\pi\varepsilon_0}$

$$\mathcal{E}(\gamma) = \mathrm{Tr}\, -\tfrac{1}{2}\Delta\gamma + \tfrac{1}{2} D(\rho_\gamma - \rho^{nuc}, \rho_\gamma - \rho^{nuc})$$

Coulomb interaction

$\rho_\gamma(x) = \gamma(x,x)$

integral kernel of γ

$$D(f,g) = \iint \frac{f(x)\, g(y)}{|x-y|}\, dx\, dy = 4\pi \int \frac{\overline{\hat{f}(q)}\, \hat{g}(q)}{|q|^2}\, dq$$

minimize over

$$\mathcal{P}^N = \{ \gamma \text{ bdd self-adjoint operators on } L^2(\mathbb{R}^3) : \; 0 \le \gamma \le 1, \; \mathrm{Tr}\,\gamma = N_{el}, \; \mathrm{Tr}\, -\tfrac{1}{2}\Delta\gamma < \infty \}$$

one-body density matrices
(closed convex hull of set of orthogonal projectors of rank N_{el}, finite KE)

$\gamma = \sum_{n=1}^{N_{el}} |\varphi_n\rangle\langle\varphi_n|$
$\Leftrightarrow \Psi = \varphi_1 \wedge \cdots \wedge \varphi_{N_{el}}$

($\exists$ minimizer γ $!\rho_\gamma$ [Solovej 1991] for neutral or positively charged systems $N_{el} \le \sum_k Z_k$)

$$\left({}^{HF} \quad \mathcal{E}^{HF}(\gamma) = \mathcal{E}(\gamma) - \tfrac{1}{2} \iint \frac{|\gamma(x,y)|^2}{|x-y|}\, dx\, dy \right)$$

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rHF periodic systems

[Catto, Le Bris, Lions 2001]

$\mathbb{L}$ lattice

Ω unit cell

$\mathbb{L}^*$ reciprocal lattice

Ω^* Brillouin zone

$$L^2 = \int_{\Omega^*}^{\oplus} L^2_\xi(\Omega)\, d\xi$$

$$\{u \in L^2_{loc} \mid \tau_k u(x) = e^{-ik\xi} u(x)\}$$

$u(x-k)$

$$\gamma = \frac{1}{(2\pi)^3} \int_{\Omega^*} \gamma_\xi \, d\xi \qquad \gamma_\xi \text{ bdd self-adjoint on } L^2_\xi$$

(missing details)

$$\rightsquigarrow \mathcal{E}_{per}(\gamma) = \frac{1}{(2\pi)^3} \int_{\Omega^*} \mathrm{Tr}_{L^2_\xi(\Gamma)} -\tfrac{1}{2}\Delta\gamma_\xi \, d\xi$$

$$+ \tfrac{1}{2} \tilde{D}(\rho_\gamma - \rho^{nuc}, \rho_\gamma - \rho^{nuc})$$

minimise over periodic set of 1-particle density matrices w/

$$\int_\Omega \rho_\gamma = N_{el}$$

charge per unit cell

$\left(\iint f(x)\, G_\Gamma(x-y)\, g(y)\, dx\, dy \right.$ where G_Γ Green's function of Poisson interaction, periodic $\left. \right)$

$\exists\, \gamma^0_{per}$ minimiser, all minimisers share density ρ^0_{per}

[Cancès, Deleurence, Lewin 2008]

Lagrange multiplier for ⊛ , [Nier, 1993]

Fermi-Dirac $f_T(\varepsilon) = \dfrac{1}{1+e^{\varepsilon/T}}$, $T>0$

$$\left[\begin{array}{l} \gamma^0_{per} = f_T(H^0_{per} - \mu^0) \\ -\Delta V^0_{per} = 4\pi(\rho^{nuc}_{per} - \rho^0_{per}) \\ \rho^0_{per} = \mathrm{den}\, \gamma^0_{per} \\ H^0_{per} = -\tfrac{1}{2}\Delta + V^0_{per} \end{array}\right.$$

Coulomb potential

$\int_\Omega \rho^0_{per} = N_{el}$ ⊛

$$f_T(\varepsilon) \xrightarrow[T\to 0]{} \mathbb{1}_{(-\infty,0]}(\varepsilon)$$

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H^0_{per} $\mathbb{L}$-periodic, $V^0_{per} \in L^2_{loc}$

$\rightsquigarrow$ self-adjoint on $L^2(\mathbb{R}^3)$, domain H^2

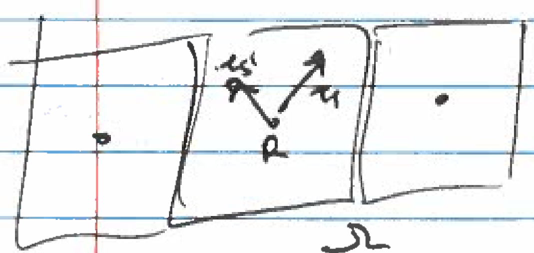
$\rightsquigarrow$ spectrum

finite temperature $T > 0$

Insulator @ $T = 0$ (with $\mu^0 \notin \sigma(-\frac{1}{2}\Delta + V^0_{per})$)

<u>Notation</u> $\rho^{nuc}(x) = \sum_{\substack{R \in \mathbb{L} \\ s=1,\dots,N_{at}}} z_s\, m(x - R - \tau_s)$

smooth cptly supported. $m \geq 0$, $\int m = 1$.



$=: \sum_{Rs} \rho^{nuc}_{Rs}(x)$

$R \in \mathbb{L}$

Force on atom Rs

$$F_{Rs} := -\int_{\mathbb{R}^3} \rho^{nuc}_{Rs}(x)\, \nabla V^0_{per}(x)\, dx$$

<u>why?</u> "Take derivative + limit"

For finite systems $T=0$:

$v_c(\rho_\gamma - \rho^{nuc})$

$$E = \mathrm{Tr}\, -\tfrac{1}{2}\Delta\gamma + \tfrac{1}{2} D(\rho_\gamma - \rho^{nuc}, \rho_\gamma - \rho^{nuc})$$

$$= \underbrace{\mathrm{Tr}\, H^0_{per} f_0(H^0_{per})}_{\sum_n \varepsilon_n f_0(\varepsilon_n)} - \cancel{\int (\rho_\gamma - \rho^{nuc}) V^0_{per}} + \tfrac{1}{2} D(\rho_\gamma - \rho^{nu}, \rho_\gamma - \rho^{nu})$$

$$- \int \rho^{nuc} V^0_{per}$$

$$\frac{\partial E}{\partial R_s} = \sum_n \langle \psi_n | \frac{\partial H^0_{per}}{\partial R_s} | \psi_n \rangle f_0(\varepsilon_n)$$

$$- \int (\rho_\gamma - \rho^{nuc}) \frac{\partial V^0_{per}}{\partial R_s} - \int \frac{\partial \rho^{nu}}{\partial R_s} V^0_{per} - \int \rho^{nu} \frac{\partial V}{\partial R_s}$$

$$= \cancel{\int \rho_\gamma \frac{\partial V^0_{per}}{\partial R_s}} - \int \cancel{(\rho_\gamma - \rho^{nu})} \frac{\partial V^0_{per}}{\partial R_s} \boxed{- \int \frac{\partial \rho^{nu}}{\partial R_s} V^0_{per}} \ \cancel{\int \rho^{nu} \frac{\partial V_{per}}{}}$$

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~~Fredholm~~

$$\cancel{T \to 0 \ : \ |e_{RS,R'S'}|}$$

Perturb nuclei distribution by displacement d

$$\nu^d := \sum_{R,S} Z_s \left[m(\cdot - R - \tau_s - d_{RS}) - m(\cdot - R - \tau_s) \right]$$

$$d \in \ell^1(\mathbb{L} \times \{1, \dots, N_{at}\}) \implies \nu^d \in L^1 \cap L^\infty$$

$\rightsquigarrow$ Defect potential $V^d_{def} := -v_c \nu^d$

where $\left[\begin{array}{l} v_c \rho := \int \frac{\rho(y)}{|\cdot - y|} dy \quad \text{"Coulomb potential operator"} \\ \widehat{v_c \rho}(q) = \frac{4\pi}{|q|^2} \hat{\rho}(q) \end{array} \right.$

Defect problem

$$V^d_{tot} = V^d_{def} + v_c \underbrace{\left(\mathrm{den}\, f_T(H^0_{per} + V^d_{tot}) - \rho^0_{per} \right)}_{=: G(V^d_{tot})}$$

$$\boxed{\begin{array}{c} \text{Levitt 2020} \\ \exists!_0 \text{ solution}, T > 0 \\ \text{for small } \nu^d \in H^{-2} \\ \implies V^d_{tot} \in L^2 \\ \text{(perturbative)} \end{array}}$$

$$\boxed{\begin{array}{c} \text{Cancès Lewin 2010} \\ \exists! V^d_{tot} \in \sqrt{v_c} L^2 \ \sim \mathcal{C}' \text{ dual of Coulomb space} \\ \text{(variational)} \end{array}}$$

Fixed point problem

$$V_{n+1} = V_n + \alpha \frac{-\Delta}{1-\Delta} \left(V^d_{def} + v_c G(V_n) - V_n \right)$$

~~Fixed~~ Kerker

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Forces $F^d_{RS} := \int_{\mathbb{R}^3} \nabla \rho^{nuc}_{RS}(x - d_{RS}) \, (V^0_{per} + V^d_{tot}) \, dx$

$$C_{RS, R'S'} := \frac{\partial F^d_{RS}}{\partial d_{R'S'}}\Big|_{d=0} \in \mathbb{R}^{3\times 3} \quad \text{IFCs}$$

Theorem $d \mapsto F^d_{RS}$ well-defined in a nbh of 0 in ℓ^1, differentiable at zero.

For $(R,S) \neq (R',S')$

$$[C_{RS,R'S'}]_{\alpha\beta} = Z_S Z_{S'} \left\langle \frac{\partial m}{\partial x_\alpha}(\cdot - R - \tau_S), W \frac{\partial m}{\partial x_\beta}(\cdot - R' - \tau_{S'}) \right\rangle$$

Screened Coulomb operator

Proof By Cancès/Lewin + Levitt

$T = 0$: $\mathcal{C} \to \mathcal{C}'$
$T > 0$: $H^{-2} \to L^2$

$$V^d_{tot} = V^d_{def} + v_c \chi_0 V^d_{tot} + O(\|\nu^d\|^2_Y) \text{ in } X$$

$(X,Y) = (\mathcal{C}', \mathcal{C})$ $T=0$

$(X,Y) = (L^2, H^{-2})$ $T>0$

"independent particle susceptibility"
= derivative of $V \mapsto \mathrm{den}\, f_T(H^0_{per} + V)$ @ 0.

$$\Rightarrow \quad V^d_{tot} = -(\epsilon^{-1} v_c)\, \nu^d + O(\|d\|^2_{\ell^1})$$

where W

$\epsilon = 1 - v_c \chi_0$
"dielectric operator"

$\|\nu^d\|_Y \lesssim \|d\|_{\ell^1}$

$$\frac{\partial V^d_{tot}}{\partial d_{R'S'}} = -W \frac{\partial \nu^d}{\partial d_{R'S'}} = W \nabla \rho^{nuc}_{R'S'}(\cdot - d_{R'S'})$$

$(R,s) \neq (R',s')$

$$C_{Rs,R's'} = \int \nabla \rho^{nuc}_{Rs} \left. \frac{\partial V^{d}_{tot}}{\partial d_{R's'}} \right|_{d=0} \quad \epsilon^{-1} v_c$$

$$= \int \nabla \rho^{nuc}_{Rs} \, W \, \nabla \rho^{nuc}_{R's'} \qquad \square$$

Theorem
$T > 0$ $\quad |C_{Rs,R's'}| \lesssim e^{-\gamma |R-R'|}$

c.f. TB results

Theorem
$T = 0$ insulators

$$C_{Rs,R's'} = -\, Z_s^{*\,T} \, \nabla^2 \boxed{\Phi_M} (R-R'+\tau_s-\tau_{s'}) \, Z_{s'}^{*} + O(|R-R'|^{-4})$$

as $|R-R'| \to \infty$

"Born effective charges"

dielectric screened Coulomb interaction
Green's function of $-\nabla \cdot (\varepsilon_M \nabla V) = 4\pi \rho$

$\varepsilon_M \in \mathbb{R}^{3\times 3}_{sym}$, $\varepsilon_M \geq 0$
macroscopic dielectric const.

Remarks
* ignoring electrons
$\chi_0 = 0$, $W = v_c$, $\varepsilon_M = 1$
$Z_s^* = Z_s$
* sum rule $\sum_s Z_s^* = 0$
so faster decay for simple lattices.

(Metals @ zero temp Friedel Oscillations
come back to later!)

e.g. $\epsilon^{-1} \frac{1}{|x|} \approx \frac{\sin(2k_F|x| + \frac{\pi}{2})}{|x|^3}$

Proof Dynamical Matrix

$$C_{RsR's'} = C_{ss'}(R-R') \longleftrightarrow D_{ss'}(q)$$

periodic

$$= \frac{1}{\sqrt{|\mathbb{L}^*|}} \sum_{R\in\mathbb{L}} C_{ss'}(R)\, e^{iqR}$$

DECAY $\longleftrightarrow$ SMOOTHNESS

~~$D_{ss'}(q) = \frac{1}{\sqrt{|\mathbb{L}^*|}}$~~

Recall

$$C_{Rs,R's'} = \langle \nabla \rho^{\text{nuc}}_{Rs}, W \nabla \rho^{\text{nuc}}_{R's'} \rangle_{L^2}$$

Fourier space?

$$Z_s\, m(\cdot - R - \tau_s)$$

Bloch transform

unitary operator $L^2(\mathbb{R}^3) \longrightarrow \boxed{L^2_{qp}(\mathbb{R}^3, L^2_{per})}$

$u \longmapsto u_\bullet$

$$(e_G, u_k)_{L^2_{per}} = \hat{u}(k+G)$$

$$\frac{1}{\sqrt{|\Omega|}} e^{iG\cdot x}$$

$$u_{k+G}(x) = e^{-iG\cdot x} u_k(x) \quad \forall G \in \mathbb{L}^*$$

$$(u_\bullet, v_\bullet) = \int_{\Omega^*} (u_k, v_k)_{L^2_{per}}$$

W $\mathbb{L}$-periodic

$\Longrightarrow \exists$ fiber decomposition $(Wu)_k = W_k u_k$

operator on L^2_{per}

$$\widehat{Wu}(k+G) = \sum_{G'\in\mathbb{L}^*} \boxed{W_{GG'}(k)}\, \hat{u}(k+G')$$

Bloch matrix

$$= (e_G, W_k e_{G'})_{L^2_{per}}$$

$Z_s\, m(\cdot - R - \tau_s)$

$$D_{ss'}(q) = \sum_{R\in\mathbb{L}} e_{ss'}(R)\, e^{iqR}$$

$$= \left\langle \sum_{R\in\mathbb{L}} e^{-iq\cdot R}\, \nabla\rho^{\mathrm{mic}}_{Rs},\ W\, \nabla\rho^{\mathrm{mic}}_{0s'} \right\rangle_{L^2}$$

$$= \int_{\mathbb{R}^3} \sum_{R\in\mathbb{L}} e^{-iq\cdot R}\, \overline{\widehat{\nabla\rho^{\mathrm{mic}}_{Rs}}(k)}\, \widehat{W\nabla\rho^{\mathrm{mic}}_{0s'}}(k)\, dk$$

$$= \int_{\Omega^*} \sum_{\substack{R\in\mathbb{L}\\ G,G'\in\mathbb{L}}} \boxed{e^{-i(q-k)\cdot R}}\, \overline{\widehat{\nabla\rho^{\mathrm{mic}}_{0s}}(k+G)}\, W_{GG'}(k)\, \widehat{\nabla\rho^{\mathrm{mic}}_{0s'}}(k+G')\, \boxed{dk}$$

$$= \delta(q-k)\,|\Omega^*|$$

$$\boxed{D_{ss'}(q) = |\Omega^*| \sum_{G,G'\in\mathbb{L}^*} \overline{\widehat{\nabla\rho^{\mathrm{mic}}_{0s}}(q+G)}\, \boxed{W_{GG'}(q)}\, \widehat{\nabla\rho^{\mathrm{mic}}_{0s'}}(q+G')}$$

Finite temperature analytic for $T>0$

Analytic away from 0 for $T=0$, insulators

$$[\epsilon^{-1}]_{GG'}(q)\,\underbrace{[v_c]_{GG'}(q)}_{\delta_{GG'}\frac{4\pi}{|q+G|^2}}$$

$$(\epsilon_q = 1 - v_{c,q}\boxed{\chi_{0,q}})$$

$$\lim_{q\to 0} [\chi_0]_{00}(q) = -\mathrm{DOS}$$

$$= \sum_{n=1}^{\infty} \int_{\Omega^*} f_T'(\varepsilon_{nk} - \mu^0)\, dk$$

Finite temperature DOS > 0

$$\Rightarrow [\chi_0]_{00}(q) \approx \text{const.}$$

$$W_{00}(q) \approx \frac{1}{1+\frac{4\pi}{|q|^2}\text{DOS}} \frac{1}{|q|^2}$$

Smooths out singularity of this

ANALYTIC $\longrightarrow$ screening

Insulators $[\chi_0]_{00}(q) \approx -q^T L q$

$$W_{00}(q) \approx \frac{1}{1+\frac{4\pi}{|q|^2} q^T L q} \frac{1}{|q|^2}$$

$$\approx \frac{1}{q^T(1+4\pi L)q}$$

$$= \frac{1}{q^T \epsilon_M q}$$

SINGULARITY $\longrightarrow$ partial screening.

Proof (more details)

Finite $T>0$

$-\chi_{0,q} + v_{c,q}^{-1}$ self-adjoint, positive w/

$$W_q = \left(-\chi_{0,q} + v_{c,q}^{-1}\right)^{-1} : L^2_{per} \to L^2_{per} \quad \text{bdd}$$

$q \mapsto W_q$ analytic in a strip $\mathbb{R}^3 + i[-a,a]^3$

$$\updownarrow \qquad (Wu)_{q+iq'} = W_{q+iq'}\, \underbrace{u_{q+iq'}}_{\frac{1}{\sqrt{|\mathcal{B}|}} \sum_R u(x+R)\, e^{-iq\cdot(x+R)}\, e^{q'\cdot(x+R)}}$$

$w_a := e^{a\sqrt{1+|x|^2}}$

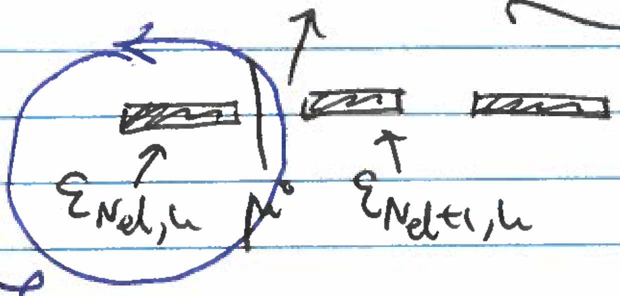
$w_{-a} W w_a$ bdd on L^2 (i.e. $W : L^2_a \to L^2_a$)

$$|C_{Rs,0s'}| \lesssim \|w_a \nabla m(\cdot - R - \tau_s)\|_{L^2}\, \|w_{-a} \nabla m(\cdot - \tau_{s'})\|_{L^2}$$
$$\lesssim e^{-\gamma|R|} \qquad \square$$

Zero temperature insulators

$$H_k^0 = -\tfrac{1}{2}\Delta_k + V_{per}^0 = \tfrac{1}{2}(-i\nabla + k)^2 + V_{per}^0$$

$\rightsquigarrow (\varepsilon_{nk}, u_{nk}) \leftarrow$ onb. of L^2_{per} of eigenfunctions of H_k^0



$$f_0(H_{per}^0 + V) = \oint_{\mathcal{C}} \left(z - H_{per}^0 - V\right)^{-1} \frac{dz}{2\pi i}$$

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$$\chi_0 V = \mathrm{den} \oint_{\mathscr{C}} (z - H^0_{per})^{-1} V (z - H^0_{per})^{-1} \frac{dz}{2\pi i}$$

derivative of
$V \mapsto \mathrm{den}\, f_0(H^0_{per} + V)$
@ $V=0$

Recall $\chi_{0\,GG'}(q) = (e_G, \chi_{0q} e_{G'})_{L^2_{per}}$

$$\rightsquigarrow \chi_{0\,GG'}(q) = \oint_{\mathscr{C}} \fint_{\Omega^*} \mathrm{Tr}_{L^2_{per}} \left[\overline{e_G}\, R_{z,k+q}\, e_{G'}\, R_{z,k} \right] dk \frac{dz}{2\pi i}$$

where
$$R_{z,k} := (z - H^0_k)^{-1}$$

(expand in (u_{nk}))

$$= \boxed{\oint_{\mathscr{C}}} \fint_{\Omega^*} \sum_{nm} \frac{\langle e_G u_{mk}, u_{nk+q}\rangle \langle u_{nk+q}, e_{G'} u_{mk}\rangle}{(z - \varepsilon_{nk+q})(z - \varepsilon_{mk})} dk \frac{dz}{2\pi i}$$

$$= \fint_{\Omega^*} \sum_{nm} \frac{f_0(\varepsilon_{nk+q}) - f_0(\varepsilon_{mk})}{\varepsilon_{nk+q} - \varepsilon_{mk}} \langle e_G u_{mk}, u_{nk+q}\rangle \langle u_{nk+q}, e_{G'} u_{mk}\rangle\, dk$$

"Adler-Wiser sum over states"

* $q \mapsto \chi_{0q}$ analytic $\Omega^* \to \mathcal{L}(L^2_{per})$

* $[\chi_{0q}]_{0G}(0) = [\chi_0]_{G0}(0) = 0$

orthonormality of u_{nk}

$$\nabla [\chi_0]_{00}(q=0) = \oint_{\mathscr{C}} \fint_{\Omega^*} \mathrm{Tr}\, \overline{e_0}\, R_{zk}\, \nabla_k H^0_k\, R_{zk}\, e_0\, R_{zk}\, dk \frac{dz}{2\pi i}$$

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$$= 0 \quad \text{"only have poles of order 3"}$$

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Therefore

$$\chi_{0,q} = \begin{bmatrix} -\frac{1}{4\pi} q^T L q + O_a(|q|^3) & B^* \cdot q + O_a(|q|^2) \\ B \cdot q + O_a(|q|^2) & \chi_{0q}^{\neq 0} \end{bmatrix}$$

where $O_a(|q|^n)$ is an analytic quantity with first $n-1$ derivatives $= 0$ @ $q=0$.

$$W_q = (-\chi_{0,q} + v_{c,q}^{-1})^{-1}$$

$$= \begin{bmatrix} -\frac{1}{4\pi} q^T (1+L) q + O_a(|q|^3) & -B^* \cdot q + O_a(|q|^2) \\ -B \cdot q + O_a(|q|^2) & -\chi_{0q}^{\neq 0} + (v_{c,q}^{\neq 0})^{-1} \end{bmatrix}^{-1}$$

Schur $\frac{4\pi}{q^T \varepsilon_M q + O_a(|q|^3)} \left[\begin{pmatrix} 1 & b^* \cdot q \\ b \cdot q & (b \cdot q) \otimes (b^* \cdot q) \end{pmatrix} + \begin{pmatrix} 0 & O_a(|q|^2) \\ O_a(|q|^2) & O_a(|q|^3) \end{pmatrix} \right]$

$$M = \begin{pmatrix} a & \overline{b}^T \\ b & D \end{pmatrix}$$

$$M/_D := a - \overline{b}^T D^{-1} b$$

$$M^{-1} = \begin{bmatrix} M/D & -(M/D)\, \overline{b}^T D^{-1} \\ -D^{-1} b (M/D) & D^{-1} + D^{-1} b (M/D)^{-1} \overline{b}^T D^{-1} \end{bmatrix}$$

$$= \frac{4\pi\, w_G(q)\, \overline{w_G(q)}}{q^T \varepsilon_M q + O_a(|q|^3)} \qquad w_G(q) = \begin{cases} 1 & G=0 \\ b_G \cdot q + O_a(|q|^2) & G \neq 0 \end{cases}$$

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$$D_{ss'}(q) = \sum_{G,G' \in \mathbb{L}^*} \overline{\widehat{\nabla\rho_{0,s}}(q+G)}\ \boxed{W_{GG'}(q)}\ \widehat{\nabla\rho_{0,s'}}(q+G')$$

$$= \frac{c\, e^{iq(\tau_s - \tau_{s'})}}{q^T \epsilon_M q + O_a(|q|^3)} \overline{\sum_G \overline{w_G(q)}\ \widehat{\nabla\rho_{0,s}}(q+G)\, e^{-iG\cdot\tau_s}}$$

$$\sum_{G'} \overline{w_{G'}(q)}\ \widehat{\nabla\rho_{0,s'}}(q+G')\, e^{-iG'\cdot\tau}$$

$\left(c = 4\pi\sqrt{|\Omega|}\right.$ or $\left. c/(2\pi)^3 \right)$

$$D_{ss'}(q)_{\alpha\beta} = c\, e^{iq\cdot(\tau_s - \tau_{s'})} \frac{\overline{\left(\sum_\gamma q_\gamma Z^*_{s,\gamma\alpha}\right)} \left(\sum_\delta q_\delta Z^*_{s,\delta\beta}\right) + O_a(|q|}{q^T \epsilon_M q + O_a(|q|^3)}$$

$$Z^*_{s,\alpha\beta} := Z_s\left[\delta_{\alpha\beta} + (2\pi)^{3/2} \sum_{G\neq 0} \overline{(b_G)}_\alpha\, c_{\beta,1}\, \hat{m}(G)\, e^{-iG\cdot\tau_s}\right.$$

"Born effective charges"

$$C_{\alpha s, \beta s'} = \int_{\mathbb{R}^3} e^{iq\cdot(\tau_s - \tau_{s'})}\, \eta(q) \underbrace{\frac{\overline{\sum_\gamma q_\gamma Z^*_{s,\gamma\alpha}} \sum_{\gamma'} q_{\gamma'} Z^*_{s',\gamma'\beta} + O_a(}{q^T \epsilon_M q + O_a(|q|^3)}}_{f(q)}$$

smooth cut off near $q=0$

Leading order term

$$f(q) = \boxed{\frac{\overline{\sum_\gamma q_\gamma Z^*_{s\gamma\alpha}} \sum_\delta q_\delta Z^*_{s'\delta\beta}}{q^T \epsilon_M q}} + \sum_{n=1}^{N-1} \frac{p_n(q)}{(q^T \epsilon_M q)^N}$$

$|R - R'|^{-(N-1)}$ term

$+ \boxed{C^{N-1} \text{ function}}$

homogeneous poly. degree $(n+2N)$

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Fact: $\widehat{f \circ A} = \dfrac{\hat{f} \circ A^{-T}}{|\det A|}$

Leading order term

"Two derivatives of $\left(|q^T \epsilon_M q|^{-1}\right)^{\vee}$"

$$\left(|\sqrt{\epsilon_M}\, q|^{-2}\right)^{\vee}(x) = \frac{\check{|\cdot|^{-2}}\,(\epsilon_M^{-1/2} x)}{\sqrt{|\det \epsilon_M|}}$$

$$= \frac{c}{\sqrt{|\det \epsilon_M|}} \frac{1}{|\epsilon_M^{-1/2} x|}$$

$$= \frac{c}{\sqrt{|\det \epsilon_M|}} \frac{1}{|x^T \epsilon_M^{-1} x|^{1/2}} = \Phi_M(x)$$

"Homogeneous term"

$\sum_{n=1}^{N-1} \dfrac{p_n(q)}{(q^T \epsilon_M q)^N}$ $\rightsquigarrow$ change of variables

$$g_n(q) = \frac{p_n(q)}{|q|^{2N}}$$

g_n locally integrable $\longrightarrow$ tempered distribution

Claim $\check{g}_n(x) = c\left(p_n(-i\nabla)|\cdot|^{2N-3}\right)(x)$

(see paper page 14)

Zero temperature metals

e.g. Free electron gas : $\epsilon_k = |k|^2$

$$\chi_0(q) = \int \frac{f_0(\epsilon_{k+q}) - f_0(\epsilon_k)}{\epsilon_{k+q} - \epsilon_k} \, dk$$

radial, <0, finite value at 0

$$= \dots = -u(q/k_F)$$

Lindhard function

not smooth @ $k = 2k_F$

$k_F \sim \sqrt{\epsilon_F}$

$$\epsilon^{-1} \frac{1}{|x|} = \int \boxed{W(q)} \, e^{i q \cdot x} \, dq$$

$$W(q) = \frac{4\pi}{|q|^2 - 4\pi \chi_0(q)}$$

$$= \dots = \frac{\sin\left(2k_F|x| + \frac{\pi}{2}\right)}{|x|^3}$$

So expect slower decay than finite temperature case

$\longrightarrow$ decay depends on smoothness of Fermi surface

e.g. Mihaila 2011