EPI and Strong Correlations in HTSC

- VIII Training Course -
- Vietri sul Mare (Salerno) Italy, 2003 -

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I. Theory of EPI

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II. Hubbard Model and HTSC

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III. 1/N Expansion for U $=\infty$

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IV. Renormalization of EPI by Strong Correlations in HTSC

↓

V. Eliashberg Equations in Strongly Correlated Superconductors

I. Theory of EPI

- Quasiparticle self-energy $\Rightarrow$ general many body theory of EPI (**GEP**)

$\downarrow$

- Low-energy physics (**LEGEP**)

small ω_D/E_F, $1/k_F l$, T_c/E_f $\Rightarrow$ simplification of GEP theory

$\downarrow$

- Limitations of Fröhlich Hamiltonian $\Rightarrow$ phonon spectra incorrect; bare vs renormalized coupling

$\downarrow$

- LDA (DFT) approach to EPI

$\downarrow$

- Inadequacy of LDA for HTSC $\Rightarrow$ local **vs** nonlocal potential

Quasiparticle Self-Energy

↓

- Hamiltonian of the system

$\Rightarrow$ electrons + lattice

↓

$$H = H_e + H_l + H_{el} \qquad (1)$$

↓

- Electrons

↓

$$H_e = \int d^3 r \hat{\psi}^\dagger(\mathbf{r}) \epsilon_0(\hat{p}) \hat{\psi}(\mathbf{r}) +$$

$$+ \frac{1}{2} \int d^3 r d^3 r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) V_c(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}'), \qquad (2)$$

↓

$$\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}') \qquad (3)$$

↓

$\epsilon_0(\hat{p}) = \hat{p}^2/2m$ - kinetic energy of electron

$V_c(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}$ - Coulomb **e-e** interaction

- Lattice Hamiltonian

↓

$$H_l = H_l^{harm} + H_l^{anh}$$

↓

$$H_l^{harm} = \frac{1}{2}\sum_n M(\frac{d\hat{\mathbf{u}}_n}{dt})^2 + \frac{1}{2}\sum_{n,m,\alpha} V_{ii}(\mathbf{R}_n^0 - \mathbf{R}_m^0) + \frac{1}{2}\sum_{n,m,\alpha}(\hat{u}_{\alpha n} - \hat{u}_{\alpha m})\nabla_\alpha V_{ii}(\mathbf{R}_n^0 - \mathbf{R}_m^0) + \frac{1}{2}\sum_{n,m,\alpha,\beta}(\hat{u}_{\alpha n} - \hat{u}_{\alpha m})(\hat{u}_{\beta n} - \hat{u}_{\beta m})\nabla_\alpha\nabla_\beta V_{ii}(\mathbf{R}_n^0 - \mathbf{R}_m^0) \quad (4)$$

↓

$V_{ii}(\mathbf{R}_n^0 - \mathbf{R}_m^0) = \frac{Z^2e^2}{|\mathbf{R}_n^0 - \mathbf{R}_m^0|}$ - bare ion-ion interaction

↓

$\hat{\boldsymbol{u}}_n = \mathbf{R}_n - \mathbf{R}_n^0$ - displacement operator

↓

H_l^{anh} - anharmonic terms with respect to $\hat{u}_n^\beta$.

↓

- Electron-lattice (ion) interaction

↓

$$H_{el} = \sum_n \int d^3 r [V_{el}(\mathbf{r} - \mathbf{R}_n^0) + \hat{\Phi}(\mathbf{r})] \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

(5)

↓

$V_{el}(\mathbf{r} - \mathbf{R}_n^0) = -\frac{Ze^2}{|\mathbf{r} - \mathbf{R}_n^0|}$ - electron-ion potential

$\hat{\Phi}(\mathbf{r})$ - **distortion operator** nonlinear in $\hat{\mathbf{u}}_n$

↓

$$\begin{aligned} \hat{\Phi}(\mathbf{r}) &= \sum_n [V_{el}(\mathbf{r} - \mathbf{R}_n^0 - \hat{\mathbf{u}}_n) - V_{el}(\mathbf{r} - \mathbf{R}_n^0)] \\ &= \hat{\Phi}^{harm}(\mathbf{r}) + \hat{\Phi}_{anh}(\mathbf{r}) \\ &= -\sum_{n,\alpha} \hat{u}_{\alpha n} \nabla_\alpha V_{e-i}(\mathbf{r} - \mathbf{R}_n^0) \\ &\quad + \frac{1}{2} \sum_{n,\alpha,\beta} \hat{u}_{\alpha n} \hat{u}_{\beta n} \nabla_\alpha \nabla_\beta V_{e-i}(\mathbf{r} - \mathbf{R}_n^0) + \ldots \end{aligned}$$

(6)

Dynamical equations for electrons and lattice

↓

How to determine electron and lattice dynamics ?

Answer: Baym-Kadanoff method $\Rightarrow$ external potentials $U(1)$, $U_\Phi(1)$

↓

$$\int d\tau H_{ext} = \int d1[U(1)\hat{\psi}^\dagger(1)\hat{\psi}(1) + U_\Phi(1)\hat{\Phi}(1)]. \quad (7)$$

↓

- introduce an **effective potential** $U_{eff}(1)$

↓

$$U_{eff}(1) = U(1) + V_H + V_{el}(1) + \langle\hat{\Phi}(1)\rangle, \quad (8)$$

↓

$$V_H = V_c(1-\bar{1})[\langle\hat{n}(\bar{1})\rangle_U - \langle\hat{n}(\bar{1})\rangle_{U=0}], \quad (9)$$

↓

$V_H^0(1) = V_c(1-\bar{1})\langle\hat{n}(\bar{1})\rangle_{U=0}$ - Hartree potential

$\hat{n}(1)$ - electron density operator

$\langle\hat{n}(1)\rangle_U$ - average for $U(1) \neq 0$

↓

$$V_{el}(1) \equiv \sum_n V_{el}(\mathbf{r} - \mathbf{R}_n^0). \qquad (10)$$

↓

- electron (**G**) and phonon (**D**) Green's functions

↓

$$G_U(1,2) = -\langle T\hat{\psi}(1)\hat{\psi}^\dagger(2)e^{-\int d\tau H_{ext}}\rangle$$
$$= [G_0^{-1}(1,2) - \hat{\Sigma}(1,2)]^{-1} \qquad (12)$$

↓

$$\tilde{D}(1,2) = -\langle T\hat{\Phi}(1)\hat{\Phi}(2)e^{-\int d\tau H_{ext}}\rangle$$
$$= [\tilde{D}_0^{-1}(1,2) - \tilde{\Pi}(1,2)]^{-1} \qquad (13)$$

↓

$G_0(1,2)$, $\tilde{D}_0(1,2)$ - **bare Green's functions**

↓

$$G_0^{-1}(1,2) = [(-\frac{\partial}{\partial \tau_1} - \epsilon_0(\mathbf{p}_1) + \mu) - U_{eff}(1) - V_H^0(1)]\delta(1-2) \quad (14)$$

↓

$\hat{\Sigma}(1,2)$, $\tilde{\Pi}(1,2)$ - **electron and phonon self-energies**

↓

How to calculate $\Sigma(1,2)$, $\Pi(1,2)$?

↓

- **vertex** function Γ_{eff}

↓

$$\Gamma_{eff}(1,2;3) = -\frac{\delta G^{-1}(1,2)}{\delta U_{eff}(3)} \quad (15)$$

↓

Γ_{eff} - electronic screening beyond the "RPA"

- "RPA" screening is due to $\delta V_H/\delta U_{eff}$

↓

- electronic self-energy $\Rightarrow$ (**see Fig**$^{(1)}$.Σ)

↓

- put $U(1) \to 0$

↓

$$\Sigma(1,2) = -V_{eff}(1,\bar{1})G(1,\bar{2})\Gamma_{eff}(\bar{2},2;\bar{1}). \tag{16}$$

↓

$V_{eff}(1,\bar{1})$ - effective retarded electronic potential

↓

$$V_{eff}(1,2) = V_c(1-\bar{1})\varepsilon_e^{-1}(\bar{1},2) + \varepsilon_e^{-1}(1,\bar{1})\tilde{D}(\bar{1},\bar{2})\varepsilon_e^{-1}(\bar{2},2), \tag{17}$$

↓

$\varepsilon_e(1,2)$ - **electronic dielectric function**

↓

$$\varepsilon_e^{-1}(1,2) = \delta(1-2) + V_c(1-\bar{1})P(\bar{1},\bar{2})\varepsilon_e^{-1}(\bar{2},2), \quad (18)$$

↓

$P(1,2)$ - irreducible electronic polarization

↓

$$P(1,2) = \frac{\delta n(1)}{\delta U_{eff}(2)} = G(1,\bar{2})\Gamma_{eff}(\bar{2},\bar{3};2)G(\bar{3},1^+) \quad (19)$$

↓

- functional equation for $\hat{\Gamma}_{eff}(1,2;3)$

↓

$$\Gamma_{eff}(1,2;3) = \delta(1-2)\delta(1-3) + \frac{\delta\Sigma(1,2)}{\delta G(\bar{1},\bar{2})} G(\bar{1},\bar{3})\Gamma_{eff}(\bar{3},\bar{4};3)G(\bar{4},\bar{2}) \quad (20)$$

↓

$\Rightarrow$ **see Fig.**Γ

↓

- **total dielectric function** $\varepsilon_{tot}(1,2)$

↓

$$\varepsilon_{tot}^{-1}(1,2) = \frac{\delta U_{eff}(1)}{\delta U(2)} = \varepsilon_{e}^{-1}(1,2) + \varepsilon_{l}^{-1}(1,2) \quad (21)$$

↓

- self-energy via $\varepsilon_{tot}(1,2)$

↓

$$\Sigma(1,2) = -V_c(1,\bar{3})\varepsilon_{tot}^{-1}(\bar{3},\bar{1})G(1,\bar{2})\Gamma_{eff}(\bar{2},2;\bar{1}) \quad (22)$$

↓

- **quasiparticle spectrum** $\omega_{\mathbf{k}}$

↓

$$G^{-1}(\mathbf{k},\omega) = 0$$

$$\omega_{\mathbf{k}} - (\frac{\mathbf{k}^2}{2m} - \mu) - \Sigma(\mathbf{k},\omega_{\mathbf{k}}) = 0 \quad (23)$$

LATTICE DYNAMICS

↓

- assume **harmonic phonons**
($1 \equiv \{\tau_1, \mathbf{R}_{n,1}\}$)

↓

- non-standard definition of phonon Green's function

↓

$$\tilde{D}(1,2) = \nabla_{\bar{\alpha}} V_{el} D_{\bar{\alpha}\bar{\beta}} \nabla_{\bar{\beta}} V_{el} \qquad (24)$$

↓

- standard phonon Green's function

↓

$$D_{\alpha\beta}(1,2) = -\langle T\hat{u}_\alpha(1)\hat{u}_\beta(2)\rangle. \qquad (25)$$

↓

DYSON EQUATION $\Rightarrow$ see Fig.D

↓

$$D^{-1}_{\alpha\beta}(1,2) = D^{-1}_{0,\alpha\beta}(1,2) - \Pi_{\alpha\beta}(1,2). \qquad (26)$$

↓

$\hat{D}_0^{-1}$ - inverse bare phonon Green's function

↓

$$\hat{D}_0^{-1}(1,2) = [M\frac{\partial^2}{\partial\tau_1^2} + U_\Phi^\alpha(1)]\delta(1-2)\hat{1} - C(1-2)$$

(27)

$$C_{\alpha\beta}(1-2) = \delta(\tau_1-\tau_2)\frac{\partial^2 V_{ii}(\mathbf{R}^0_{n_1} - \mathbf{R}^0_{n_2})}{\partial R^0_{\alpha,n_1}\partial R^0_{\beta,n_2}}$$

$$-\delta(1-2)\sum_{n_3\neq n_1}\frac{\partial^2 V_{ii}(\mathbf{R}^0_{n_1} - \mathbf{R}^0_{n_3})}{\partial R^0_{\alpha,n_1}\partial R^0_{\beta,n_3}}$$

(28)

↓

- phonon self-energy $\Pi_{\alpha\beta}(1-2)$

↓

$$\Pi_{\alpha\beta}(1-2) =$$

$$\int d\mathbf{r}_3 d4\chi(\mathbf{r}_3\tau,4)\nabla_\alpha V_{el}(\mathbf{r}_3 - \mathbf{R}^0_{n_1})\nabla_\beta V_{el}(\mathbf{r}_4 - \mathbf{R}^0_{n_2}) -$$

$$\delta_{n_1 n_2} \sum_{n_3 \neq n_1} \int d\mathbf{r}_3 d\mathbf{r}_4 \chi(\mathbf{r}_3 \tau, \mathbf{r}_4 \tau^+) \nabla_\alpha \times$$

$$V_{el}(\mathbf{r}_3 - \mathbf{R}^0_{n_1}) \nabla_\beta V_{el}(\mathbf{r}_4 - \mathbf{R}^0_{n_3}) \qquad (29)$$

↓

- **charge susceptibility** $\chi_c(1,2)$

↓

$$\chi_c(1,2) = P(1,\bar{2}) \varepsilon_e^{-1}(\bar{2},2) \qquad (30)$$

↓

- **phonon spectrum** (and life-time)

$$\det D^{-1}_{\alpha\beta}(\mathbf{k},\omega) = 0. \qquad (31)$$

↓

Discussion

- Functional equations for G, Γ_{eff}, D, P
- Practically impossible solution
- How to simplify the problem?

LOW-ENERGY PHYSICS (LEGEP)

↓

- **small** ω_D/E_F, $1/k_f l$)

↓

- adiabatic approximation due to $\frac{\omega_D}{E_F} << 1$

⇓

MIGDAL THEOREM $\Rightarrow \Sigma$ is linear in D

↓

$$\Gamma_{eff}(1,2;3) \cong \Gamma_c(1,2;3) + \delta\Gamma_{ep}(1,2;3) \qquad (32)$$

↓

$$\delta\Gamma_{ep}(1,2;3) = \frac{\delta\Sigma_{EP}(1,2)}{\delta u_{eff}(3)} \qquad (33)$$

↓

$\Rightarrow$ **see Fig**. **Migdal**

↓

- pure electronic vertex $\Gamma_c(1,2;3)$

↓

$$\Gamma_c(1,2;3) = \delta(1-2)\delta(1-3) + \frac{\delta\Sigma_c(1,2)}{\delta u_{eff}(3)} \quad (34)$$

↓

- **total self-energy** $\Sigma(1,2)$

↓

$$\Sigma(1,2) = \Sigma_c(1,2) + \Sigma_{ep}(1,2) \quad (35)$$

↓

- electronic part of self-energy $\Sigma_c(1,2)$

↓

$$\Sigma_c(1,2) \approx -V_c^{sc}(1,\bar{1})G(1,\bar{2})\Gamma_c(\bar{2},2;\bar{1}), \quad (36)$$

↓

$V_c^{sc}(1,2)$ - screened Coulomb interaction

↓

$$V_c^{sc}(1,2) = V_c(1,\bar{2})\varepsilon_e^{-1}(\bar{2},2) \quad (37)$$

↓

- EPI self-energy $\Sigma_{ep}(1,2)$

$$\downarrow$$

$$\Sigma_{ep}(1,2) = -V_{ep}(\bar{1},\bar{2})\Gamma_c(1,\bar{3};\bar{1})G(\bar{3},\bar{4})\Gamma_c(\bar{4},2;\bar{2}), \quad (38)$$

$$\downarrow$$

$V_{ep}(1,2)$ - screened EPI interaction

$$\downarrow$$

$$V_{ep}(1,2) = \varepsilon_e^{-1}(1,\bar{1})\nabla V_{el}(\bar{1})D(\bar{1},\bar{2})\nabla V_{el}(\bar{2})\varepsilon_e^{-1}(\bar{2},2) \quad (40)$$

$$\downarrow$$

- Low energy physics $\Rightarrow$ high energy processes should be integrated out

$$\Downarrow$$

renormalized parameters g, λ, m^*

$$\downarrow$$

$$G(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - (\mathbf{k}^2/2m - \mu) - \Sigma(\mathbf{k},\omega_n)}$$

$$\downarrow$$

$$= G^{low}(\mathbf{k},\omega_n) + G^{high}(\mathbf{k},\omega_n) \quad (41)$$

$$= O(s^{-1}) + O(s^0)$$

↓

ω_c and δk_c **separate small** $s \ll 1$ from s^0

↓

- definition small

↓

$$s \ll \delta k_c/k_F \ll 1$$

$$s \ll \omega_c \ll 1 \qquad (42)$$

↓

- analogous separation for phonons

↓

$$D^{low}(\mathbf{k}, \omega_n) \sim s^0, \quad D^{high}(\mathbf{k}, \omega_n) \sim s^2. \qquad (43)$$

↓

- note $M \sim m(E_F/\omega_{ph})^2 \sim s^{-2}$

$D_{00} \sim 1/M\omega_n^2 \sim s^2$, $\omega_n \sim \omega_c$ and $D_{00} \sim 1$, $\omega_n \ll \omega_c$

↓

- further simplification:Coulomb part $\Sigma_c(1,2)$

↓

$$\Sigma_c(1,2) = \Sigma_c^{(0)}(1,2) + \Sigma_c^{(1)}(1,2), \tag{44}$$

↓

$\Sigma_c^{(0)} \sim s^0$ and $\Sigma_c^{(1)} \sim s$.

↓

- for further purposes define Σ_0

↓

$$\Sigma_0(1,2) = \{U(1) + V_{el}(1) + V_H(1)\}\delta(1-2) + \Sigma_c^{(0)}(1,2). \tag{45}$$

↓

- note U, V_{e-i}, $V_H \sim s^0$

↓

- Fourier transform with respect to time (and for small ω_n) $\Rightarrow \Sigma_0$

↓

$$\Sigma_0(\mathbf{x},\mathbf{y},\omega_n) \simeq \Sigma_0(\mathbf{x},\mathbf{y},0) + \Sigma_0'(\mathbf{x},\mathbf{y},0) \bullet i\omega_n. \tag{46}$$

↓

- **note** $\Sigma_0' \bullet \omega_n \sim s^1$ because $\omega_n \sim s^1$

↓

- **note** $\Sigma_c^{(1)}(1,2)$ contains $G^{low}(1,2)$

↓

- **similar analysis** holds for $\Sigma_{ep}(1,2) \sim s$

↓

- **separations o**f terms s^0 **and** s^1

⇓

LOW-ENERGY DYSON EQUATION

↓

$$[i\omega_n Z_c(\mathbf{x},\bar{\mathbf{x}}) - H_0(\mathbf{x},\bar{\mathbf{x}}) - \Sigma_c^{(1)}(\mathbf{x},\bar{\mathbf{x}},\omega_n)$$

$$- \Sigma_{ep}(\mathbf{x},\bar{\mathbf{x}},\omega_n)] \times G^{low}(\bar{\mathbf{x}},\mathbf{y},\omega_n) = \delta(\mathbf{x}-\mathbf{y}), \quad (47)$$

↓

high-energy processes in $Z_c(\mathbf{x},\mathbf{y})$, $H_0(\mathbf{x},\mathbf{y})$

↓

$$Z_c(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}) - \Sigma_0'(\mathbf{x},\mathbf{y},0), \quad (48a)$$

↓

$$Z_c(\mathbf{x},\bar{\mathbf{z}})Z_c^{-1}(\bar{\mathbf{z}},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}) \quad (48b)$$

↓

$$H_0(\mathbf{x},\mathbf{y}) = (-\frac{1}{2m}\nabla_{\mathbf{x}}^2 - \mu)\delta(\mathbf{x}-\mathbf{y}) + \Sigma_0(\mathbf{x},\mathbf{y},0) \quad (49)$$

↓

- renormalized Green's function G^{ren}

↓

$$G^{ren}(x,\mathbf{y},\omega_n) = Z_c^{1/2}(\mathbf{x},\bar{\mathbf{x}})G^{low}(\bar{x},\bar{\mathbf{y}},\omega_n)Z_c^{1/2}(\bar{\mathbf{y}},\mathbf{y}) \quad (50)$$

↓

- ideal band-structure Hamiltonian $h_0(x,\mathbf{y})$

↓

$$h_0(x,\mathbf{y}) = Z_c^{-1/2}(\mathbf{x},\bar{\mathbf{x}})H_0(\bar{x},\bar{\mathbf{y}},\omega_n)Z_c^{-1/2}(\bar{\mathbf{y}},\mathbf{y})$$

$$h_0(x,\mathbf{y}) = (-\frac{1}{2m}\nabla^2_{\mathbf{x}} - \mu)\delta(\mathbf{x}-\mathbf{y}) + V_{ren}(\mathbf{x},\mathbf{y}). \quad (51)$$

↓

- many-body excitation nonlocal (crystal) potential $V_{ren}(\mathbf{x},\mathbf{y})$

↓

$$V^{ren}(\mathbf{x},\mathbf{y}) = \Sigma_0(\mathbf{x},\mathbf{y},0) + \delta T(\mathbf{x},\mathbf{y}) \quad (52)$$

$$\delta T(\mathbf{x},\mathbf{y}) = Z_c(\mathbf{x},\bar{\mathbf{y}})T_0(\bar{\mathbf{y}},\bar{\mathbf{z}})Z_c^{-1}(\bar{\mathbf{z}},\mathbf{y}) - T_0(\mathbf{x},\mathbf{y}) \quad (53)$$

↓

- electron ”kinetic energy” $T_0(\mathbf{x},\mathbf{y})$

↓

$$T_0(\mathbf{x},\mathbf{y}) = (-\frac{1}{2m}\nabla^2_{\mathbf{x}} - \mu)\delta(\mathbf{x}-\mathbf{y}) \qquad (54)$$

↓

- $V^{ren}(\mathbf{x},\mathbf{y})$ meaningful for $\delta k \ll k_F$

↓

- LDA potential $V_{S-H}(\mathbf{x},\mathbf{y}) \neq V^{ren}(\mathbf{x},\mathbf{y})$! (**see latter**)

↓

- define **quasiparticle vertex** function Γ^{ren}

↓

$$\Gamma^{ren}(1,2;3) = Z_c^{-1/2}\Gamma_c Z_c^{-1/2} \qquad (55)$$

↓

- renormalized self-energies $\Sigma^{ren}_{c,ep}$

↓

$$\Sigma^{ren}_{c,ep}(x,\mathbf{y},\omega_n) = Z_c^{-1/2}(\mathbf{x},\bar{\mathbf{x}})\Sigma^{ren}_{c,ep}(\bar{x},\bar{\mathbf{y}},\omega_n)Z_c^{-1/2}(\bar{\mathbf{y}},\mathbf{y}). \qquad (56)$$

DYSON EQUATION FOR $G^{ren}(\chi, \mathbf{y}, \omega_n)$

$\downarrow$

$$[i\omega_n \delta(\mathbf{x} - \bar{\mathbf{x}}) - h_0(\mathbf{x}, \bar{\mathbf{x}}) - \Sigma_c^{(1)ren}(\mathbf{x}, \bar{\mathbf{x}}, \omega_n)$$

$\downarrow$

$$- \Sigma_{ep}^{ren}(\mathbf{x}, \bar{\mathbf{x}}, \omega_n)] G^{ren}(\bar{\mathbf{x}}, \mathbf{y}, \omega_n) = \delta(\mathbf{x} - \mathbf{y}) \hat{\tau}_0, \quad (57)$$

$\downarrow$

$\Sigma_c^{(1),ren}$, Σ_{ep}^{ren} look like Σ_c, Σ_{ep} in $Eqs.(36 - 38)$

$\downarrow$

but with G, Γ_c replaced by G^{ren}, Γ_c^{ren}

LEGEP method

↓

- **project** high-energy into low-energy sector

↓

- **find** the ideal band structure spectra $\xi_i(\mathbf{p})$

↓

$$h_0(\mathbf{x}, \bar{\mathbf{y}})\Psi_{i,\mathbf{p}}(\bar{\mathbf{y}}) = \xi_i(\mathbf{p})\Psi_{i,\mathbf{p}}(\mathbf{x}). \quad (58a)$$

↓

- **expand** $G^{ren}(\bar{\mathbf{x}}, \mathbf{y}, \omega_n)$, Γ^{ren}, ε_e, ∇V_{el} in basis $\Psi_{i,\mathbf{p}}(\mathbf{x})$

↓

- write down **Eliashberg equations** in **basis** $\Psi_{i,\mathbf{p}}(\mathbf{x})$

↓

- LEGEP is **never realized** for strongly correlated systems !

↓

- vertex $\Gamma^{ren}(1,2;3)$ and $\varepsilon_e(1,2)$ are unknown

↓

-* LEGEP is **partly** realized in t-J-EP model

↓

- $\xi_i(\mathbf{p})$ different from LDA spectrum

↓

$$\xi_i(\mathbf{p}) \neq \xi_i^{LDA}(\mathbf{p}) \qquad (58b)$$

↓

- in weakly correlated s,p-metals **Na**, **Mg**, **Al**

$$\Downarrow$$

$$\xi_i(\mathbf{p}) \approx \xi_i^{LDA}(\mathbf{p})$$

Limitations of the Fröhlich model

↓

- most papers treat EPI in the Fröhlich model!

- assume monoatomic (**with mass M**) unit cell (with 1e/cell)

- **case T=0 K**

↓

$$\mathbf{u}_n(0) = i\sum_{\mathbf{q},\lambda}\left(\frac{\hbar}{2NM\omega^{(0)}_{\mathbf{q},\lambda}}\right)^{1/2}\mathbf{e}_{\mathbf{q},\lambda}\left(b_{\mathbf{q}\lambda} + b^{\dagger}_{-\mathbf{q}\lambda}\right)e^{i\mathbf{q}\mathbf{R}^0_n}$$

(59)

↓

$$H_{Fr} = \sum_{\mathbf{k},\sigma}\xi_{0,\mathbf{k}} f^{\dagger}_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + \sum_{\mathbf{q},\lambda}\omega_0\left(b^{\dagger}_{\mathbf{q}\lambda} b_{\mathbf{q}\lambda} + \frac{1}{2}\right)$$

↓

$$+ \sum_{\mathbf{k},\sigma,\mathbf{q},\lambda} g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}} f^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} f_{\mathbf{k}\sigma}\left(b^{\dagger}_{-\mathbf{q}\lambda} + b_{\mathbf{q}\lambda}\right)$$

(60)

↓

ASSUMPTIONS (to simplify calculation)

↓

- bare" isotropic spectrum $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$

- "**bare**" dispersionless phonons $\omega^{(0)}_{\mathbf{q},\lambda} = \omega_0$

- no explicit Coulomb interaction

- "bare" EPI coupling $g^0_{\mathbf{k},\mathbf{k}+\mathbf{q}} \approx g_0$

↓

- Renormalized phonon Green's function $D(\mathbf{q}\lambda, \omega)$

↓

$$D(\mathbf{q}\lambda, \omega) = -i < 0 \mid T(B_{\mathbf{q}\lambda}(t) B^{\dagger}_{\mathbf{q}\lambda}(0) \mid 0 >_{\omega} \qquad (61)$$

$$B_{\mathbf{q}\lambda} = b_{\mathbf{q}\lambda} + b^{\dagger}_{-\mathbf{q}\lambda}$$

↓

- "bare" Green's function $D_0(\mathbf{k}, \omega)$

↓

$$D_0(\mathbf{q}\lambda, \omega) = \frac{2\omega_0}{\omega^2 - \omega_0^2 + i\eta} \qquad (62)$$

↓

- Eqs.(28-31) for $D^{-1}(q\lambda) = D_0^{-1} - \Pi$

but $V_c = 0$

↓

-define $q \equiv (\mathbf{q}, \omega)$

$$D(q) = \frac{2\omega_0}{\omega^2 - \omega_0^2[1 + \lambda_0 P_0(q)/N(0)]} \qquad (63)$$

↓

- ”bare” EPI coupling constant λ_0

↓

$$\lambda_0 = 2N(0)\frac{g_0^2}{\omega_0} \qquad (64)$$

- polarization operator $P_0(q)$

↓

$$P_0(q) = -2i\int \frac{d^4p}{(2\pi)^4} G_0(p)G_0(p+q) \qquad (65)$$

↓

$\lim_{\mathbf{q}\to 0,\omega\to 0} P_0(q) = -N(0)$

↓

- phonon spectrum $\omega_{ren}(\mathbf{q})$ for $\mathbf{q} \to 0$

$$\omega_{ren} = \omega_0 \sqrt{1 - \lambda_0} \qquad (66)$$

↓

- lattice stability $\Rightarrow \omega_{ren}^2 \geq 0 \Rightarrow \lambda_0 \leq 1$!

↓

- electron Green's function for $\omega \ll \omega_0$

↓

$$G(k, \omega) = \frac{(1+\lambda)^{-1}}{\omega - \xi_k - i\delta sign(k - k_F)} \qquad (67)$$

↓

- renormalized quasiparticle spectrum ξ_k

↓

$$\xi_k = \frac{\xi_{0,k}}{1+\lambda} \qquad (68)$$

↓

- effective mass $m^* = m(1+\lambda)$

↓

- for weekly q-dependence $P_0(\mathbf{q}) \sim P_0(0)$

$\Downarrow$

$$\lambda \approx \frac{\lambda_0}{1-\lambda_0} \qquad (69)$$

$\downarrow$

- the renormalized coupling λ is measurable quantity

- note for $\lambda_0 \to 1$ one has $\lambda \to \infty \quad \Longrightarrow$ no limitations on λ !!

$\downarrow$

CONCLUSIONS

$\downarrow$

- the ”bare” EPI coupling λ_0 is **undefined quantity** $\Longrightarrow$ Coulomb interaction is not taken into account

$\downarrow$

- phonon spectra **can not** be calculated in the Fröhlich model

- most conclusions in the Fröhlich model on the limiting value of $\lambda < 1$ **are unfounded**

- in PbBi alloys $\lambda = 2.5$!

LDA (DFT) approach to EPI

↓

$$H\{\rho_e(\mathbf{r})\} = T + V_c + V_{el} \qquad (70)$$

↓

$$V_{el} = \sum_{i=1}^{N_e} V_{el}(\mathbf{r}_i), \quad V_{el}(\mathbf{r}_i) = \sum_{\alpha} V_{el}(\mathbf{r}_i - \mathbf{R}_\alpha) \qquad (71)$$

↓

- $H\{\rho_e(\mathbf{r})\}$ with **non-degenerate ground state** $|\ \Psi_g\rangle$

↓

$$|\ \Psi_g\rangle = |\ \Psi_g\{\rho_e(\mathbf{r})\}\rangle \qquad (72)$$

↓

- Ground state functional $E\{\rho_e(\mathbf{r}); V_{el}(\mathbf{r})\}$

↓

$$E\{\rho_e(\mathbf{r}); V_{el}(\mathbf{r})\} = \langle \Psi_g\{\rho_e(\mathbf{r})\} \ |\ H\{\rho_e(\mathbf{r})\} \ |\ \Psi_g\{\rho_e(\mathbf{r})\}\rangle. \qquad (73)$$

↓

- Hohenberg-Kohn theorem (at $T = 0\ K$)

↓

$\Rightarrow$ | $\Psi_g\rangle$ and $E\{\rho_e(\mathbf{r}); V_{ei}(\mathbf{r})\}$ unique functionals on $\rho_e(\mathbf{r})$ for given $V_{el}(\mathbf{r})$

↓

↓

$$E\{\rho_e(\mathbf{r})\} = F\{\rho_e(\mathbf{r})\} + \int d^3r \rho_e(\mathbf{r}) V_{el}(\mathbf{r}). \quad (74)$$

↓

- $F\{\rho_e(\mathbf{r})\}$ is unknown functional

⇓

APPROXIMATIVE SCHEME

↓

- Kinetic energy functional of free electrons

↓

$$T_0\{\rho_e(\mathbf{r})\} = \langle \Psi_{0g}\{\rho_e(\mathbf{r})\} \mid T \mid \Psi_{0g}\{\rho_e(\mathbf{r})\}\rangle, \quad (75a)$$

↓

↓

- Free-electron ground state

$$| \ \Psi_{0g}\{\rho_e(\mathbf{r})\}\rangle \ = \det[\Psi_k(\mathbf{r}_i)], \tag{75b}$$

↓

$$\rho_e(\mathbf{r}) = \sum_k \ | \ \Psi_k(\mathbf{r}) \ |^2 \tag{75c}$$

- the exchange-correlation term $E_{XC}\{\rho_e(\mathbf{r})\}$ picks up correlations beyond Ha

↓

$$F\{\rho_e(\mathbf{r})\} \ = T_0\{\rho_e(\mathbf{r})\} \ + \frac{1}{2}\int d^3r \int d^3r' \, \frac{\rho_e(\mathbf{r})\rho(\mathbf{r}')}{| \ \mathbf{r}-\mathbf{r}' \ |}$$

↓

-Minimum of $E\{\rho_e(\mathbf{r}); V_{ei}(\mathbf{r})\}$

↓

$$\frac{\delta T_0\{\rho_e(\mathbf{r})\}}{\delta\rho_e(\mathbf{r})} + V_{ei}(\mathbf{r}) + V_H(\mathbf{r}) + V_{XC}(\mathbf{r}) = \mu, \tag{77}$$

↓

$$V_H(\mathbf{r}) = \int d^3r' \frac{\rho(\mathbf{r}')}{\mid \mathbf{r} - \mathbf{r}' \mid}, \quad V_{XC}(\mathbf{r}) = \frac{\delta E_{XC}}{\delta \rho_e(\mathbf{r})} \tag{78}$$

↓

μ - chemical potential

↓

- $\Psi_k(\mathbf{r})$ solution of the Kohn-Sham equation

↓

$$[\frac{\hat{\mathbf{p}}^2}{2m} + V_g(\mathbf{r})]\Psi_k(\mathbf{r}) = \epsilon_k \Psi_k(\mathbf{r}), \tag{79}$$

↓

- The g**round state** potential $V_g(\mathbf{r})$

↓

$$V_g(\mathbf{r}) = V_{el}(\mathbf{r}) + V_H(\mathbf{r}) + V_{XC}(\mathbf{r}) \tag{80}$$

↓

↓

↓

- The unknown exchange-correlation energy $E_{XC}\{\rho_e(\mathbf{r})\}$ **nonlinear** and **nonlocal** quantity of $\rho_e(\mathbf{r})$

LOCAL DENSITY APPROXIMATION (*LDA*)

$\Downarrow$

$\Downarrow$

E_{XC} is **local**

$\downarrow$

$$E_{XC}\{\rho_e(\mathbf{r})\} \approx \int\int d^3r \rho_e(\mathbf{r}) \varepsilon_{XC}(\rho_e(\mathbf{r})), \quad (81)$$

$\downarrow$

- Hedin-Lundquist interpolation formula for $V_{XC}(\mathbf{r})$

$\downarrow$

$$V_{XC}(\mathbf{r}) \approx -1.5\alpha(\rho_e(\mathbf{r}))(3\rho_e(\mathbf{r})/\pi)^{1/3}, \quad (82)$$

$\downarrow$

- **Ground-state energy**

$E_g\{V_{el}(\mathbf{r})\} = \min E\{\rho_e(\mathbf{r}); V_{el}(\mathbf{r})\}$

$\downarrow$

$$E_g\{V_{el}(\mathbf{r})\} = \sum_{k=1}^{N_e} \epsilon_k^{LDA} +$$

$$+\frac{1}{2}\int d^3r\rho_e(\mathbf{r})[-V_H(\mathbf{r})-2V_{XC}(\mathbf{r})+2\varepsilon_{XC}(\rho_e(\mathbf{r}))] \quad (83)$$

↓

- The spectrum ϵ_k^{LDA} is an **auxiliary quantity** by which E_g is calculated

↓

- ϵ_k^{LDA} is in principle not quasiparticle excitation energy

↓

- **Ideal band-structure** is due to $h_0(x,\mathbf{y})$ (see Eqs.51-58)

↓

- EPI is dynamical effect due to excited squasiparticles

↓

- In practice the LDA band structure is calculated and used for EPI

↓

How to calculate EPI in LDA?

↓

- ”Phonons” $\Rightarrow$ $V_g \rightarrow V_g + \delta V_g$

↓

$$\delta V_g(\mathbf{r}) = \sum_n \frac{\delta V_g(\mathbf{r}-\mathbf{R}_n)}{\delta \mathbf{R}_n}\mathbf{u}_n \qquad (84)$$

↓

$$\frac{\delta V_g(\mathbf{r}-\mathbf{R}_n)}{\delta \mathbf{R}_n} = \nabla V_{ei}(\mathbf{r}-\mathbf{R}_n)$$

$$+\left[\frac{\delta V_H(\mathbf{r})}{\delta \rho_e(\bar{\mathbf{r}})} + \frac{\delta V_{XC}(\mathbf{r})}{\delta \rho_e(\bar{\mathbf{r}})}\right]\frac{\delta \rho_e(\bar{\mathbf{r}})}{\delta \mathbf{R}_n}. \qquad (85)$$

↓

- linear response theory

↓

$$\mathbf{P}_n(\mathbf{r}) = \frac{\delta \rho_e(\mathbf{r})}{\delta \mathbf{R}_n} = \chi_c(\mathbf{r},\bar{\mathbf{r}})\frac{\delta V_{ei}(\bar{\mathbf{r}}-\mathbf{R}_n)}{\delta \mathbf{R}_n}$$

$$= \chi_c^0(\mathbf{r},\bar{\mathbf{r}})\frac{\delta V_g(\bar{\mathbf{r}}-\mathbf{R}_n)}{\delta \mathbf{R}_n}, \qquad (86)$$

↓

- (Non)interacting χ_c^0 (and χ_c) charge susceptibility

↓

- static *LDA* ”vertex” function Γ_{LDA}

↓

$$\Gamma_{LDA}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') + \frac{\delta V_{XC}(\mathbf{r})}{\delta\rho_e(\bar{\mathbf{r}})}\chi_c^0(\bar{\mathbf{r}},\bar{\mathbf{r}}_1)\Gamma_{LDA}(\bar{\mathbf{r}}_1,\mathbf{r}') \quad (87)$$

↓

$$\frac{\delta V_g(\mathbf{r}-\mathbf{R}_n)}{\delta\mathbf{R}_n} = \Gamma_{LDA}(\mathbf{r},\bar{\mathbf{r}})\varepsilon_e^{-1}(\bar{\mathbf{r}},\bar{\mathbf{r}}_1,0)\nabla V_{ei}(\bar{\mathbf{r}}_1-\mathbf{R}_n). \quad (88)$$

↓

The *LDA* static $\varepsilon_e(\mathbf{r},\mathbf{r}',0)$

↓

$$\varepsilon_e^{-1}(\mathbf{r},\mathbf{r}',0) = \delta(\mathbf{r}-\mathbf{r}') + V_c(\mathbf{r}-\bar{\mathbf{r}})\chi_c(\bar{\mathbf{r}},\mathbf{r}'), \quad (89)$$

↓

$$\chi_c(\mathbf{r},\mathbf{r}') = \chi_c^0(\mathbf{r},\mathbf{r}') + [V_c(\mathbf{r}-\bar{\mathbf{r}}) + \frac{\delta V_{XC}(\mathbf{r})}{\delta\rho_e(\bar{\mathbf{r}})}]\chi_c^0(\bar{\mathbf{r}},\bar{\mathbf{r}}_1)\chi_c(\bar{\mathbf{r}}_1,\mathbf{r}') \quad (90)$$

↓

↓

- *LDA EPI* coupling constant $g^{(LDA)}_{\alpha,ll'}$

↓

$$g^{(LDA)}_{\alpha,ll'}(\mathbf{k},\mathbf{k}') = \sum_n g^{(LDA)}_{\alpha,nll'}(\mathbf{k},\mathbf{k}')$$

$$= \langle \psi_{\mathbf{k}l} \mid \sum_n \frac{\delta V_g(\mathbf{r})}{\delta R_{n\alpha}} \mid \psi_{\mathbf{k}'l'} \rangle \quad (91)$$

↓

- $g^{(LDA)}_{\alpha,ll'}(\mathbf{k},\mathbf{k}')$ is due to the ground state properties

- Note, real $g_{\alpha,ll'}(\mathbf{k},\mathbf{k}')$ is determined via the excited states and nonlocal $V^{ren}(\mathbf{x},\mathbf{y})$!

- What to do with $g^{(LDA)}_{\alpha,ll'}(\mathbf{k},\mathbf{k}')$?

- In practice one uses Eliashberg equations and replaces $g_{\alpha,ll'}(\mathbf{k},\mathbf{k}') \Rightarrow g^{(LDA)}_{\alpha,ll'}(\mathbf{k},\mathbf{k}')$

- **LDA is good for phonons** which are due to ground state spectra

↓

Linear-response method for $\boldsymbol{g^{(LDA)}_{\alpha,ll'}(\mathbf{k},\mathbf{k}')}$

↓

- Instead of calculating $\Gamma_{LDA}(\mathbf{r}, \bar{\mathbf{r}}_1)$ and $\varepsilon_e^{-1}(\bar{\mathbf{r}}_1, \bar{\mathbf{r}}_2, 0)$ (difficult job)

↓

use the Kohn-Sham equation with phonons

↓

$$[\frac{\hat{\mathbf{p}}^2}{2m} + V_g^0(\mathbf{r}) + \sum_n \frac{\delta V_g^0(\mathbf{r})}{\delta \mathbf{R}_n}\mathbf{u}_n]\Psi_k(\mathbf{r})$$

$$= (\epsilon_k^0 + \sum_n \frac{\delta \epsilon_k^0}{\delta \mathbf{R}_n})\Psi_k(\mathbf{r}) \qquad (92)$$

- The solution in the form

↓

$$\Psi_k(\mathbf{r}) = \Psi_k^0(\mathbf{r}) +$$

$$+ \sum_n \frac{\delta \Psi_k^0(\mathbf{r})}{\delta \mathbf{R}_n}\mathbf{u}_n \qquad (93)$$

↓

$$[\frac{\hat{\mathbf{p}}^2}{2m} + V_g^0(\mathbf{r})]\frac{\delta \Psi_k^0(\mathbf{r})}{\delta \mathbf{R}_n}$$

$$= [\frac{\delta \epsilon_k^0}{\delta \mathbf{R}_n} - \frac{\delta V_g^0(\mathbf{r})}{\delta \mathbf{R}_n}]\Psi_k^0(\mathbf{r}) \qquad (93)$$

↓

$$\frac{\delta n(\mathbf{r})}{\delta \mathbf{R}_n} = \sum_k n_{F,k}\{\Psi_k^{0*}(\mathbf{r})\frac{\delta \Psi_k^0(\mathbf{r})}{\delta \mathbf{R}_n} + \Psi_k^0(\mathbf{r})\frac{\delta \Psi_k^{0*}(\mathbf{r})}{\delta \mathbf{R}_n}\} \qquad (94)$$

↓

- $n_{F,k}$ the Fermi function at **T=0 K**