INTERNATIONAL ATOMIC ENERGY AGENCY
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SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE

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SMALL POLARON CONDUCTION

(Lectures I & II)

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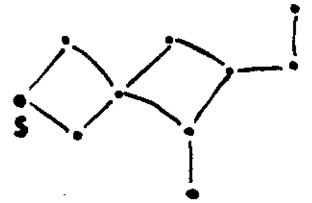
$$H_c = \sum_s \varepsilon_s c_s^+ c_s + \sum_{s,i} t_{s,i}\left(c_s^+ c_{s+i} + c_{s+i}^+ c_s\right)$$



$$H_{ph} = \sum_{q,\lambda} \hbar\omega_{q\lambda}\, b_{q\lambda}^+ b_{q\lambda}$$

$$H_{ep} = \sum_{q,\lambda,s} \hbar\omega_{q\lambda}\, \alpha_{\lambda q}^{1/2}\, i\left(b_{q\lambda} e^{i\vec{q}\cdot\vec{R}_s} - b_{q\lambda}^+ e^{-i\vec{q}\cdot\vec{R}}\right) c_s^+ c_s$$

$$\alpha_{ac}(q) = \frac{\Xi_d^2 |q|^2}{2\rho V \hbar\omega_{ac}^3(q)} \qquad \rho = \text{mass density}$$

$$\alpha_{opt}(q) = \frac{A^2}{2\bar{\rho} V \hbar\omega_{op}^3(q)} \qquad \bar{\rho} = \text{reduced mass density.}$$

1. Complete squares in Hamiltonian:

$$H = \sum_s \varepsilon_s c_s^+ c_s + \sum_{s,i} t_{s,i}\left(c_s^+ c_{s+i} + c_{s+i}^+ c_s\right)$$
$$+ \sum_{q\lambda} \hbar\omega_{\lambda q}\left[b_{q\lambda}^+ + i\alpha_{\lambda q}^{1/2} \sum_s e^{i\vec{q}\vec{R}_s} c_s^+ c_s\right]\left[b_{q\lambda} - i\alpha_{\lambda q}^{1/2} \sum_{s'} e^{-i\vec{q}R_s'} c_{s'}^+ c_{s'}\right]$$

$$- \sum_{q\lambda} \hbar\omega_{\lambda q}\, \alpha_{\lambda q} \sum_{s,s'} e^{iq(\vec{R}_s - \vec{R}_{s'})} c_s^+ c_s c_{s'}^+ c_{s'}$$

$$B_{q\lambda}^+ = b_{q\lambda}^+ + i\alpha_{\lambda q}^{1/2} \sum_s e^{i\vec{q}\vec{R}_s} c_s^+ c_s.$$

$$\ell_s^+ = c_s^+ \prod_{q\lambda} e^{i\alpha_{\lambda q}^{1/2}\left[e^{-i\vec{q}\vec{R}_s} b_{q\lambda}^+ + e^{i\vec{q}\vec{R}_s} b_{q\lambda}\right]}$$

$$\ell_s = c_s \prod_{q\lambda} e^{-i\alpha_{\lambda q}^{1/2}\left[e^{i\vec{q}\vec{R}_s} b_{q\lambda} + e^{-i\vec{q}\vec{R}_s} b_{q\lambda}^+\right]}$$

Displaced phonons and polarons.

$$c_s^+ = \ell_s^+ \prod_{q\lambda} e^{-i\alpha_{\lambda q}^{1/2}\left[e^{-i\vec{q}\vec{R}_s} b_{q\lambda}^+ + e^{i\vec{q}R_s} b_{q\lambda}\right]}$$

$$\left[\ell_s^+, \ell_{s'}\right]_+ = \delta_{s,s'}$$

$$\left[\ell_s^+, B_{q\lambda}\right]_- = 0$$

$$H = \varepsilon_s l_s^+ l_s + \sum t_{s,i} \left(l_s^+ l_{s+i} X_{s,s+i} + l_{s+i}^+ l_s X_{s+i,s} \right)$$

$$+ \sum_{q\lambda} \hbar \omega_{\lambda q} B_{q\lambda}^+ b_{q\lambda}$$

$$- \sum_{\lambda,q} \hbar \omega_{\lambda q} \alpha_{\lambda q} \sum_s l_s^+ l_s$$

$$- \sum_{\lambda,q} \hbar \omega_{\lambda q} \alpha_{\lambda q} \sum_{s,s'\neq s} e^{i\vec{q}(\vec{R}_s - R_{s'})} \, l_s^+ l_s l_{s'}^+ l_{s'}$$

$$X_{s,s+i} = \prod_{q\lambda} e^{-i\alpha_{\lambda q}^{\hbar} \left[e^{-i\vec{q}\vec{R}_s} - e^{-i\vec{q} R_{s+i}} \right] B_{q\lambda}^+ + h.c.}$$

Current operator

$$\vec{r} = \sum_s R_s c_s^+ c_s = \sum R_s l_s^+ l_s$$

$$i\hbar \dot{\vec{r}} = \sum_{s,i} t_{s,i} (\vec{R}_{s+i} - R_s) \left(c_{s+i}^+ c_s - c_s^+ c_{s+i} \right)$$

$$\vec{j} = -\frac{e}{i\hbar} \sum_{s,i} t_{s,i} (\vec{R}_{s+i} - \vec{R}_s) \left(c_{s+i}^+ c_s - c_s^+ c_{s+i} \right)$$

$$= -\frac{e}{i\hbar} \sum_{s,i} t_{s,i} (\vec{R}_{s+i} - \vec{R}_s) \left(l_{s+i}^+ l_s X_{s+i,s} - l_s^+ l_{s+i} X_{s,s+i} \right)$$

Current correlation function (App)

$$\langle \vec{j}(t) \vec{j}(0) \rangle = \sum_{s,i} \langle j(t) j(0) \rangle^{s,i}$$

$$= \frac{e^2}{\hbar^2} \sum_{s,i} t_{s,i}^2 (\vec{R}_{s+i} - \vec{R}_s)(\vec{R}_{s+i} - \vec{R}_s)$$

$$\langle l_s^+(t) l_{s+i}(t) X_{s,s+i}(t) \, l_{s+i}^+ l_s X_{s+i,s} \rangle$$

$$= \frac{e^2}{\hbar^2} \sum_{s,i} t_{s,i}^2 (\vec{R}_{s+i} - \vec{R}_s)(\vec{R}_{s+i} - R_s)$$

$$\langle l_s^+(t) l_{s+i}(t) l_{s+i}^+ l_s \rangle$$

$$\Big\{ \underbrace{\langle X_{s+i,s}(t) X_{s,s+i} \rangle - \langle X_{s+i,s} X_{s,s+i} \rangle}_{P_{s,i}(t)} + \underbrace{\langle X_{s+i,s} X_{s,s+i} \rangle}_{Q_{s,i}} \Big\}$$

$$\langle l_s^+(z)\, l_{s+i}(z)\, l_{s+i}^+\, l_s \rangle$$

$$= e^{\frac{i}{\hbar}(\epsilon_s - \epsilon_{s+i}) z}\; n_e^{(s)}\; n_h^{(s+i)}$$

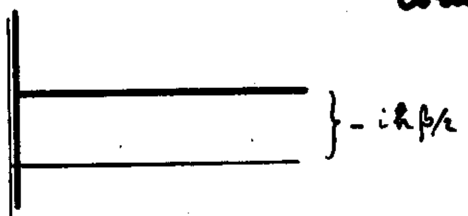
$$= e^{\frac{i}{\hbar}(\epsilon_s - \epsilon_{s+i}) z}\; \frac{e^{\beta(\epsilon_{s+i}-\epsilon_s)/2}}{4\cosh\beta\epsilon_s/2\,\cosh\beta\epsilon_{s+i}/2}$$

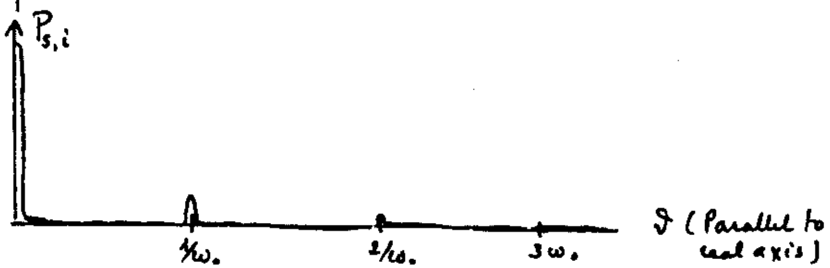
$$Q_{s,i} = e^{-2\sum \alpha_{\lambda q}\sin^2\left(\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)\right)\coth\hbar\omega_\lambda(q)\beta/2}$$

$$P_{s,i}(z) = Q_{si}\times$$

$$\left\{ e^{2\sum\alpha_{\lambda q}\sin^2\left(\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)\right)\frac{\cos\omega_{\lambda q}(z+i\hbar\beta/2)}{\sinh\hbar\omega_{\lambda q}\beta/2}} - 1\right\}$$

complex z plane





$$P^{(s,i)}(z) = Q^{(s,i)}$$

$$\exp\left\{\sum_{q\lambda}\frac{2\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)}{\sinh\hbar\omega_{\lambda q}\beta/2}\cosh\left\{\omega_{\lambda q}\left[\operatorname{Im}z+\tfrac{1}{2}\hbar\beta\right]\right\}\right.$$

$$\times\exp\left\{-i\hbar\sum\frac{2\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)}{\sinh\hbar\omega_{\lambda q}\beta/2}\,\omega_{\lambda q}\sinh\left\{\omega_{\lambda q}\left[\operatorname{Im}z+\tfrac{1}{2}\hbar\beta\right]\right\}\right.$$

$$\times\exp\left\{-\hbar^2\sum\frac{\alpha_{\lambda q}\sin^2\vec{q}/2(\vec{R}_{s+i}-\vec{R}_s)}{\sinh\hbar\omega_{\lambda q}\beta/2}\,\omega_{\lambda q}^2\cosh\left\{\omega_{\lambda q}[\quad]\right\}\right\}$$

Structure $\eta_{si} = 2\sum_{q\lambda}\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)$

$\omega_{\lambda q} = \omega_0$ (no dispersion)

$$P^{s,i} = Q_{si}\;\exp\left\{\eta^{(s,i)}\frac{1}{\sinh\hbar\omega_0\beta/2}\cosh\omega_0\left[\operatorname{Im}z+\tfrac{1}{2}\hbar\beta\right]\right\}$$

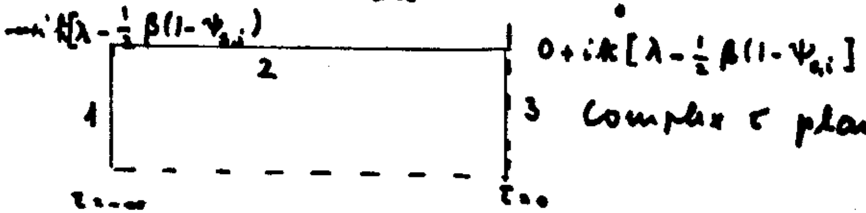
$$\times\exp\left\{-i\omega_0\hbar\;\eta^{(si)}\frac{\sinh\omega_0\left[\operatorname{Im}z+\frac{1}{2}\hbar\beta\right]}{\sinh\hbar\omega_0\beta/2}\right\}$$

$$\exp\left\{-\omega_0^2\hbar^2\;\frac{1}{2}\eta^{(s)}_{si}\frac{\cosh\omega_0\left[\operatorname{Im}z+\frac{1}{2}\hbar\beta\right]}{\sinh\hbar\omega_0\beta/2}\right\}$$

$$\langle l_s^+(z)\, l_{s+i}(z)\, l_{s+i}^+\, l_s\rangle = e^{\frac{i}{\hbar}(\epsilon_s-\epsilon_{s+i})\vartheta}\times$$

$$\frac{e^{-(\epsilon_s-\epsilon_{s+i})\frac{1}{\hbar}\left[\operatorname{Im}z+\hbar\beta/2\right]}}{4\cosh\beta\epsilon_s/2\,\cosh\beta\epsilon_{s+i}/2}$$

$$\underline{\sigma}^{(s,i)}(\omega,T) = \int_{-\infty}^{0} dt\, e^{(i\omega+s)\tau} \int_{0}^{\beta} d\lambda\, \langle \underline{j}(\tau - i\hbar\lambda)\, \underline{j}(0)\rangle^{s,i}$$



Complex τ plane

(1) $\underline{\sigma}^{(s,i)(1)}(\omega,T) = 0$

(2) $$\sigma^{(s,i)(2)}(\omega,T) = \int_{-\infty}^{0}\int_{0}^{\beta} d\vartheta\, d\lambda\, e^{[\omega+s](\vartheta + i\hbar\lambda - i\hbar\beta/2(1-\Psi_{si}))} \langle \underline{j}(\vartheta - i\hbar\beta/2(1-\Psi_{si}))\, \underline{j}(0)\rangle^{s,i}$$

Carry out the λ Integration

$$\underline{\sigma}^{(s,i)(2)}(\omega,T) = \beta\, \frac{\sinh \hbar\omega\beta/2}{\hbar\omega\beta/2}\, e^{-\frac{1}{2}\hbar\omega\beta\Psi_{si}} \int_{-\infty}^{0} e^{(i\omega-s)\vartheta} \langle \underline{j}(\vartheta - i\hbar\beta/2(1-\Psi_{si}))\, \underline{j}(0)\rangle^{si}$$

(3) $$\underline{\sigma}^{(s,i)(3)}(\omega,T) = -i\hbar \int_{0}^{\beta} d\lambda\, e^{-\hbar\omega\lambda} \int_{1/2\beta(1-\Psi_{si})}^{\lambda} d\gamma\, e^{\hbar\omega\gamma} \langle \underline{j}(-i\hbar\gamma)\, \underline{j}(0)\rangle^{si}.$$

purely imaginary.

Insert in $\underline{\sigma}^{(s,i)(2)}$

$$\underline{\sigma}^{(s,i)(2)}(\omega,T) = \beta\, \frac{\sinh \hbar\omega\beta/2}{\hbar\omega\beta/2}\, e^{-\frac{1}{2}\hbar\beta\Psi_{si}(\omega + [\varepsilon_s - \varepsilon_{s+i}]\frac{1}{\hbar})}$$

$$\frac{1}{4\cosh\beta\varepsilon_s/2\, \cosh\beta\varepsilon_{s+i}/2}$$

$$e^{-2\sum \alpha_{\lambda q} \sin^2\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)[\coth \hbar\omega_{\lambda q}\beta/2 - \frac{\cosh \hbar\omega_{\lambda q}\beta/2\, \Psi_{s,i}}{\sinh \hbar\omega_{\lambda q}\beta/2}]}$$

$$\int_{-\infty}^{0} e^{i\omega\vartheta + \frac{i}{\hbar}(\varepsilon_s - \varepsilon_{s+i})\vartheta - i\vartheta \sum \frac{2\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(R_{s+i}-R_s)}{\sinh \hbar\omega_{\lambda q}\beta/2}\omega_{\lambda q}\sinh \hbar\omega_{\lambda q}\beta\Psi_{si}/2}$$

$$e^{-\vartheta^2 \sum \frac{\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(R_{s+i}-\vec{R}_s)}{\sinh \hbar\omega_{\lambda q}\beta/2}\omega_{\lambda q}^2 \cosh \hbar\omega_{\lambda q}\beta\Psi_{si}/2} \cdot \frac{e^2}{\hbar^2} t_{si}^2 (\vec{R}_{s+i}-\vec{R}_s)(\vec{R}_{s+i}-\vec{R}_s)$$

$$\boxed{\omega + (\varepsilon_s - \varepsilon_{s+i})\frac{1}{\hbar} - \sum \frac{2\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(R_{s+i}-R_s)}{\sinh \hbar\omega_{\lambda q}\beta/2}\omega_{\lambda q}\sinh \hbar\omega_{\lambda q}\beta\Psi_{si}/2 = 0}$$

$$\int_{-\infty}^{0} e^{-\vartheta^2 A}\, d\vartheta = \frac{\sqrt{\pi}}{2A^{1/2}}$$

$$\underline{\sigma}^{(s,i)(2)}(\omega,T) = \beta\, \frac{\sinh \hbar\omega\beta/2}{\hbar\omega\beta/2}\, e^{-1/2\hbar\beta\Psi_{si}(\omega + [\varepsilon_s - \varepsilon_{s+i}]\frac{1}{\hbar})}$$

$$\frac{1}{4\cosh\beta\varepsilon_s/2\, \cosh\beta\varepsilon_{s+i}/2}\; \frac{\sqrt{\pi}}{2\left(\sum \frac{\alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(R_{s+i}-R_s)}{\sinh\frac{1}{2}\hbar\omega_{\lambda q}\beta}\omega_{\lambda q}^2 \cosh\ldots\right)^{1/2}}$$

$$\cdot\, e^{-2\sum \alpha_{\lambda q}\sin^2\frac{1}{2}\vec{q}(\vec{R}_{s+i}-\vec{R}_s)[\coth \hbar\omega_{\lambda q}\beta/2 - \frac{\cosh \hbar\omega_{\lambda q}\beta/2\,\Psi_{si}}{\sinh \hbar\omega_{\lambda q}\beta/2}]}$$

$$\frac{e^2}{\hbar^2} t_{s,i}^2 (\vec{R}_{s+i}-\vec{R}_s)(\vec{R}_{s+i}-\vec{R}_s)$$

Solution of implicit equ. High temperature

$$\omega + (\varepsilon_s - \varepsilon_{s+i})\frac{1}{\hbar} - \sum 2 \Delta\lambda_q \sin^2 \tfrac{1}{2}\vec{q}(\vec{R}_{s+i} - \vec{R}_s)\, \omega_{q\lambda}\, \Psi_{s,i}/\hbar = 0$$

$$\Psi_{s,i} = \frac{\omega + (\varepsilon_s - \varepsilon_{s+i})/\hbar}{\eta \cdot \omega_0}$$

$$\sigma^{(s,i)(2)}(\omega, T) = \sigma^{(s,i)(2)}(0,T)\, \frac{\sinh \hbar\omega\beta/2}{\hbar\omega\beta/2}\, e^{-\frac{1}{2}\hbar\beta \frac{[\omega + (\varepsilon_s - \varepsilon_{s+i})]^2}{(2)\,\eta\cdot\omega_0}}$$

$$\sigma^{(s,i)}(0,T) = \frac{e^2}{\hbar^2} t_{s,i}^2 (\vec{R}_{s+i} - \vec{R}_s)(\vec{R}_{s+i} - \vec{R}_s) \frac{\sqrt{\pi}}{4 \cosh \beta\varepsilon_s/2 \, \cosh \beta \varepsilon_{s+i}/2}$$

$$\frac{\beta}{2\left(\sum \frac{\Delta\lambda_q \sin^2 \frac{1}{2}\vec{q}(R_{s+i} - R_s)}{\sinh \hbar\omega_{\lambda q}\beta}\, \omega_{\lambda q}^2 \cosh(\,)\right)^{1/2}}$$

$$e^{-\eta \tanh \hbar\omega_0\beta/4}$$

$$= \frac{e^2}{\hbar^2} t_{s,i}^2 (\vec{R}_{s+i} - \vec{R}_s)(\vec{R}_{s+i} - \vec{R}_s) \frac{\sqrt{\pi}}{4 \cosh \beta\varepsilon_s/2 \, \cosh \beta\varepsilon_{s+i}/2}$$

$$\frac{\beta}{2\left(\frac{\eta\,\omega_0^2}{\frac{1}{2}\hbar\beta\omega_0}\right)^{1/2}}\, e^{-\eta \tanh \hbar\omega_0\beta/4}$$

$$U = \eta\, \hbar\omega_0/4$$

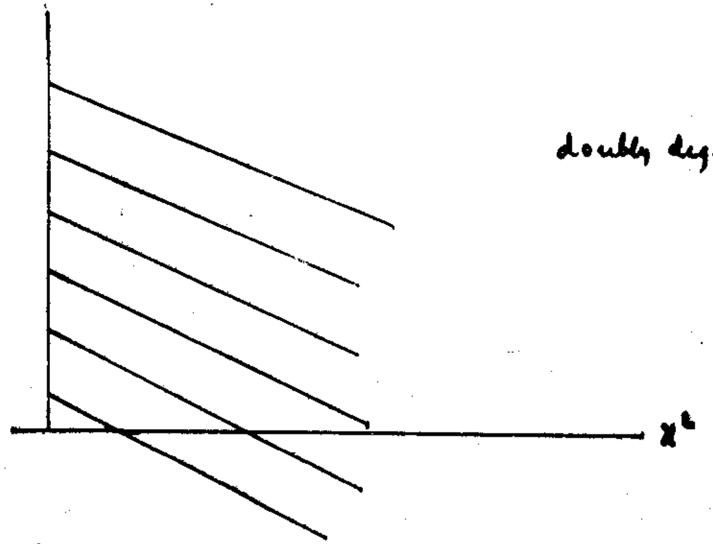
Ordered cubic

$$\sum_i (\vec{R}_{s+i} - \vec{R}_s)_\alpha (R_{s+i} - R_s)_\beta = \delta_{\alpha\beta} \frac{2a^2}{3}$$

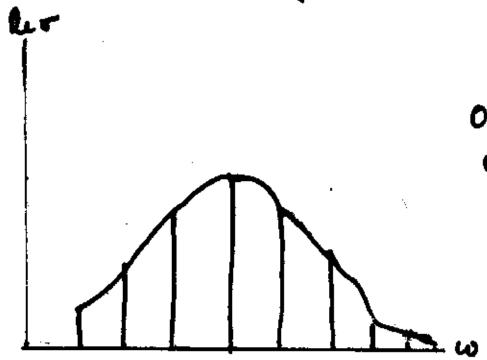
Frequency of the real part of the conductivity

$$\sim \frac{\sinh \hbar\omega\beta/2}{\hbar\omega\beta/2}\, e^{-\frac{\hbar^2(\omega + (\varepsilon_s - \varepsilon_{s+i}))^2}{16\, U\, kT}}$$

Suppose no dispersion no disorder, take two electronic levels s, s+1



doubly degenerate.



Only absorption at $n\omega$.
Consequence of model

What are the consequences if we include the effect of transfer integral in the calculation of the Polaron states?