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THEORY OF PEIERLS DISTORTION, KOHN ANOMALY AND SUPERCONDUCTING TRANSITION TEMPERATURE

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ABSTRACT

Recently seven organic conductors have shown $A=A_0\lambda e^{-b\lambda}$ *type function in UV-Visible spectra which can be related with photometallic nature and dynamic with Kohn anomaly. Other four organic and metal – organic charge transfer complexes have shown* $A(k) = A_0k\exp(-bk)$ *type function in the infrared range which can be related with Peierls distortion. Some other conductors show oscillatory behaviour of electronic conduction and light absorption against temperature, pressure and frequency which can be explained by complex band gap. The Fourier transforms are Cauchy distributions which are symmetric and the phenomena are related with the amplitude and phase modulation of charge density waves. Further consequences of such a function leading to an equation for transition temperature are presented after proving certain conditions for maximum conductivity when temperature, frequency and pressure are varied. The Gaussian bands are also analyzed to prove conditions for the Frohlich sliding mode. We get transition temperature for Frohlich super conduction.*

Keywords: ***UV-Visible And IR Spectra, Phase Modulation, Fourier Transform, Beta Density, Transition Temperature***

I. INTRODUCTION

Recently seven polyiodide chain complexes-three based on small organic molecule and four finite macromolecules or biopolymers-have shown $A=A\lambda e^{-b\lambda}$ where A is absorption in the UV-visible spectra [1, 2] TTF-TCNQ (TTF=tetrathiafulvalinium, TMTSF-DDQ (TMTSF=tetramethyl tetraselena-fulvalinium, DDQ=2,3-dichloro-5,6-dicyano-p-benzoquinone) TCNQ=7,7,8,8-tetracyano-p-quinodimethane and two CT complexes of Cu(N-CH_3-salim)$_2$ have shown [4] $A(k)=A_0ke^{-bk}$ function where k is wave number in the infrared range [3]. This behaviour was explained with Peierls instability. Present work is regarding theory of light-induced Peierls distortion [5] and Kohn anomaly [6], the concept of complex band gap which is related with dynamic Kohn anomaly [7] and over-damped cases leading to static distortion.

It is shown that function has relation with lattice distortion due to Peierls instability [8]. The function is the Erlang distribution in statistics and having symmetric Cauchy distribution due to Cauchy-distorted lattice similar to a Gaussian-distorted lattice in metal chain in metal-organic chelates like Ni $(Hdmg)_2$ where Hdmg-dimethylglyoxime under high pressure. This function is also same which appears in high pressure resistivity [9] as $\rho = \rho_0 Pe^{-bP}$ and even low temperature conductance $C=(1/R) = C_0 T e^{-bT}$ [10].

Recently light induced Peierls instability leading to $A(\lambda)=A_0\lambda e^{-b\lambda}$ function is observed in seven organic conductors. A theory of light induced Peierls distortion is developed here to interpret some of the under-damped cases (V>0) in which oscillatory behaviour of electronic conduction and light –absorption is found. In over damped cases, (V<0) b is real and the exponential fall in absorption depending on the value of b is found.

This theory is extended here to obtain breaking temperature by comparing K_BT_c with the magnetic energy or power dissipation.

II. EXPERIMENTAL

The function $A(\lambda)=A_0\lambda e^{-b\lambda}$ was found to fit in the UV-visible spectra of benzophenone-KI-I_2, deoxycholic acid-KI-I_2, lithocholic acid-KI-I_2, stearic acid-KI-I_2, tripalmitin—KI-I_2, lysozyme-KI-I_2 and folic acid – KI-I_2 [2], while in TTF-TCNQ, TMTSF-DDQ and two CT complexes of Cu $(N\text{-}CH_3\text{-}Salim)_2$ $A(K)=A_0ke^{-bk}$ was found to fit in the IR spectra [3]. This function is the same which appears in high pressure resistivity and even low temperature conductivity [6,9]. The function is recognized as Erlang distribution in statistics. The Fourier transform or spectral function is a symmetric Cauchy distribution [11] which shows there is a Cauchy distorted lattice making a linear chain inhomogeneous.

Apart from this, an oscillatory behaviour of electronic conduction and light absorption was found with temperature, pressure or frequency as variables. Benzidine-DDQ showed oscillations in resistivity vs temperature eventually band gap going to zero as in two dimensional systems [12], transition metal dichalcogenide showed oscillations in resistivity with applied pressure [13], cadmium selenide showed oscillations in absorption with wavelength, folic and folic acid-KI-I_2 showed oscillations in infrared spectra [13], metal-free phthalocyanine and its DDQ complex showed oscillations in infrared spectra [14], and resistivity of some materials showed oscillations as the applied magnetic field was increased [15]. These phenomenon of oscillations was found for imaginary and repulsive potential. Oscillations in absorption and conduction are explained with α-σ relations.

An equation is derived for second order fluctuation in phase angles which is also related with oscillator strengths. The oscillator strength is related with the first derivative spectra [16]. This is the first step towards fluctuation theory of elementary excitation. If electro magnetic (light) waves is incident, the potential energy is $\hbar\omega$, in high pressure studies V is to be replaced by elastic energy proportional to P^2 and in low temperature studies band gap changes by $E_g(T) \cong E_g(0) - \alpha T$ and it reduces to zero in 2D conductors. For V>0, there is repulsive interactions among electrons, photons and phonons then oscillations arise.

When α-cyclodextrin-KI-I_2 amylose-iodine and (coumarin)$_4$-KI-I_2 were studied for resistivity under high pressure, it showed $\rho(P) = \rho_0 P e^{-bP}$ type behaviour which is Erlang distribution. This may be due to particle-size distribution in these nano-materials or due to pressure induced Peierls distortion as explained elsewhere [8] because the Fourier transform or spectral function in deformation is symmetric Cauchy distribution. $\rho(x) = \rho_0 b / (b^2 + V'^2)$ where V′ is displacement (strain) or volume change. Benzidine-TCNQ showed beta density in conductance $C(T) = C_0 T^{*1/2}(1-T^*)^{1/2}$ under high pressure above 70 kilobars where $T^*=(T-a)/b$ in temperature range which is beta density. Some other complexes such as DTN, DTN-I_2,pyrene-$2I_2$, anthracene-TNB(trinitro benzene) and α-cyclodextrin-KI-I_2 as well as amylose-iodine (both at 1000 Kz) showed half-power and square-power beta densities with $\rho(P) = AP^{*1/2}(1-P^*)^{1/2}$ and $\rho(P) = AP^{*2}(1-P^*)^2$ where $P^* = (P-a)/b$. Here a general equation is derived for resistivity or conductivity where half=power beta density appears as amplitude modulation of charge density waves.

Apart from the above properties, some macromolecular biomolecules showed half-power beta density, i.e. $A = A_0 K^{*1/2}(1-K^*)^{1/2}$ in the infrared spectra where $K^* = (K-a)/b$, such as steric acid,stearic acid –KI-I_2, Linoleic acid-KI-I_2,Arachidonic acid – KI-I_2, tripalmitin-KI-I_2, lysozyme-KI-I_2, cytochrome c, cytochrome c – TCNQ, Cytochrome c – DDQ, Valinomycine-I_2, gramicidine-I_2, β-carotene, etc [2] which appear due to general formula for amplitude modulation of CDWs. These beta densities were explained due to polaron hopping in macromolecular solids.

Finally in the present work a Gaussian equation appearing in many metal-organic conductors in infrared range and in some organic conductors in the absence of electron-phonon resonance is used to calculate width of the Gaussian and also transition temperature for a large width Gaussian band which nearly becomes a Cauchy distribution.

III. THEORETICAL BACKGROUND

The pressure dependence of electrical resistivity of several organic conductors such as α-cyclodextrim-KI-$I_2.4H_2O$,amylose-iodine and (coumarin)$_4$-KI-I_2 as well as benzidine-TCNQ have shown $\rho = APe^{-bP}$ type function where ρ is the resistivity and P is the applied pressure. This is an Erlang distribution is statistics. It is an asymmetric curve but its Fourier transform is a Cauchy distribution which is symmetric. Considering volume as a thermodynamic conjugate volume and as a Fourier conjugate,

$$\rho(V)=\left(\frac{b/\pi}{b^2+V'^2}\right)\pi \tag{1}$$

V' is volume. Lattice distortion leads to inhomogeneous chain for charge transport. It is a Cauchy distorted lattice similar to a Gaussian distorted lattice of metal chains in Ni(Hdmg)$_2$. Nickel chains are hard metal chains, and iodine chains are soft. Cauchy distortion occurs in soft chains which can be derived as increase in width of a Gaussian.

By putting the mean free path λ to be limited to wavelength of charge density wave. λ~1/k where k is wave number of charge density wave (CDWs). Then

$$\rho=\frac{\hbar^2k^2}{ne^2\nu\hbar}=\frac{2m^*(E-V)}{ne^2\nu\hbar} \tag{2}$$

V can be screened-Coulomb potential with the Thomas-Fermi screening constant which shows that the kinetic energy of charge carriers is lost in screening the distorted lattice [8, 17].

In the UV-visible spectra of organic and biomolecular polyiodide chain complexes $A=A_0\lambda e^{-b\lambda}$ type Erlang distribution is found where λ is wavelength. The spectral function is like Drude model, because $A(k)=A_0\, b\big/\left(b^2+k^2\right)$ is similar to $\rho_{ac}=\rho_{dc}\big/\left(1+\omega^2\Im^2\right)$ due to ω=(2πc)/λ, this is equivalent to

$$\sigma_{ac}=\frac{\sigma_{dc}}{1+\left(2\pi c/\lambda\right)^2\Im^2} \tag{3a}$$

$$\sigma_{ac}=\frac{\sigma_{dc}\lambda^2}{\lambda^2+\left(4\pi^2c^2\right)\Im^2}=\frac{\sigma_{dc}\lambda^2}{\lambda^2+\lambda_0^2} \tag{3b}$$

which is free-carrier absorption in metals, with $\sigma=\frac{\alpha n_1 c}{4\pi}$.

In TTF-TCNQ, TMTSF-DDQ and charge transfer complexes of Cu(N-CH$_3$-Salim)$_2$ $A=A_0\lambda e^{-bk}$ function is found. This suggests dynamic Kohn anomaly and leads to Cauchy-distorted lattice described by $A(\lambda)=b\big/\left(b^2+\lambda^2\right)$ where λ is deformation.

3.1 Phase modulation and resistivity function

The spectral function of

$$A(\lambda)=A_0\lambda e^{-b\lambda} \text{ is } A(k)=A_0\frac{b}{b^2+k^2} \tag{4}$$

One more integration gives

$$\int\frac{b}{b^2+k^2}dk=\frac{1}{b}\tan^{-1}\frac{k}{b} \tag{5}$$

The phase angle $\Phi = \tan^{-1} - (k/b)$ is related with modulation of CDWs. Combining the above equations

$$\frac{\partial^2 \Phi}{\partial \lambda \partial k} = \left(A_0 \lambda e^{-b\lambda}\right) e^{-i\lambda k} \tag{6a}$$

The second order function Φ leads to $A_0 \lambda e^{-b\lambda}$ type function. This equation can be also written as

$$\frac{\partial^2 \Phi}{\partial \lambda \partial k} = \left(A_0 e^{-\lambda(b+ik)+\ln\lambda}\right) \tag{6b}$$

$$A = A_0 e^{\lambda\sqrt{b^2+k^2}} e^{i\Phi+\ln\lambda} \tag{7}$$

Leads to

$$A(\lambda) = A_0 \frac{b}{b^2+\lambda^2} \tag{7a}$$

Using

$$\int \frac{b}{b^2+\lambda^2} d\lambda = \frac{1}{b}\tan^{-1}\frac{\lambda}{b} \tag{7b}$$

Where $\Phi = \tan^{-1}\frac{\lambda}{b}$ is the phase angle. Then $\frac{\partial^2 \Phi}{\partial \lambda \partial k} = \left(A_0 e^{-bk}\right) e^{i\lambda k}$

$$\frac{\partial^2 \Phi}{\partial \lambda \partial k} = \left(A_0 e^{-k(b+i\lambda)+\ln k}\right) \tag{8}$$

$$A(\lambda) = A_0 e^{-k\sqrt{b^2+k^2}} e^{i\Phi+\ln k}$$

The equations 8(b) and 8(c) are the differential equations to be solved for Φ in terms of integral transforms,

$$\Phi = \int \Im(ke^{-bk})dk = \int L(ke^{-ik\lambda})d\lambda \tag{9}$$

Where $\Im$ and L are the Fourier and Laplace transforms respectively. Similarly,

$$\Phi = \int \Im(ke^{-bk})d\lambda \tag{10a}$$

$$\Phi = \int L(ke^{-ik\lambda})dk \tag{10b}$$

3.2 Light induced Peierls instability

The absorption in UV-visible light is given by $\alpha(\lambda)=\alpha_0\lambda\exp(-b\lambda)$ while it is given by $\alpha(k) = \alpha_0' \, k \exp(-bk)$ in the infrared range. A band gap due to Peierls instability opens up in the infrared range. In UV-visible range charge carriers are free and follow the Drude model. Using α - σ relation $\sigma = \alpha n_1 c/4\pi$. The conductivity is given by spectral function of $\alpha(\lambda)$.

Now we discuss Peierls distortion. The Fourier transfer transform of $A_0\lambda e^{-b\lambda}$ is

$$\rho = \frac{4\pi}{n_1 c} A_0 \left(\frac{b^2 + k^2}{b} \right) \tag{11}$$

This should be compared with

$$\rho = \frac{2m^*(E - V)}{ne^2 \nu \hbar} \tag{12}$$

By comparing constant and variable terms and solving for A_0 and b gives

$$A_0 = i\left(\frac{(ne^2\nu\hbar)(4\pi/n_1 c)k}{(2m^* E)^{1/2}(2m^* V)^{1/2}} \right) \tag{13a}$$

$$b = i\left(\frac{E}{V} \right)^{1/2} k \tag{13b}$$

The substitutions in $\sigma = \left(\frac{n_1 c}{4\pi} \right) \alpha_0 \lambda e^{-b\lambda}$ equation lead to

$$\sigma = i \frac{(ne^2\nu\hbar)}{(2m^* E)^{1/2}(2m^* V)^{1/2}} \times \lambda k \exp\left[-i\left(\frac{E}{V} \right)^{1/2} \lambda k \right] \tag{14}$$

This also proves beta density of the type $\rho \propto P^{*1/2}(1-P)^{1/2}$ and $\alpha \propto k^{*1/2}(1-k)^{1/2}$ in pressure dependence of resistivity and wave-vector dependence of absorption in infrared range which is because of amplitude modulation of charge density waves because V=(E-T) or β(P-P_0) or V=α(k-k_0) where β and α are constants. This leads to $E^{1/2}$ $V^{1/2}$=k_1 $P^{1/2}$ (P-P_0)$^{1/2}$ and $E^{1/2}$ $V^{1/2}$=$k_2 k^{1/2}$ (k-k_0)$^{1/2}$ which are beta densities. Such modulations are also found in UV-visible spectra of charge transfer complexes of lead phthacuamine and infrared spectrum of biocytine-iodine complex. There is correlated hopping occurring in hard chains lead and soft chains of iodine [18, 19].

Exactly similarly analysis of $\alpha(k) = \alpha_0' \, k \exp(-bk)$ function whose spectral function is $\alpha(\lambda) = A_0 b \big/ \left(b^2 + \lambda^2\right)$ leads to

$$A_0 = i\left(\frac{\left(ne^2\nu\hbar\right)(4\pi / n_1 c)\lambda}{(2m^* V)^{1/2}(2m^* E)^{1/2}} \right) \tag{15a}$$

$$b = \left(\frac{e}{V} \right)^{1/2} \lambda \tag{15b}$$

which are analogous to A_0 and b in equations (13a and 13b) except that λ replaces k. Substitution in conductivity leads the same equation (14).

The imaginary A_0 and b shows that oscillations in conductivity and absorbance are possible V>0. When V<0, A_0 and b are real. In that case, we observe sharp rise in λ and k linearly and then exponentially falling for large λ and k. A_0 describes amplitude modulation while b describes phase modulation of CDWs.

In an idealized metal, a free electron gas follows $\in(q) \cong 1+\lambda^2/q^2$ in the limit $q \to 0$.

The oscillatory behaviour can be explained with complex band gap. $E_g=E_c+iE_i$ where E is the electronegativity difference. $E_i = \hbar\omega_i = \hbar\nu_g(k_1+ik_2)$.Thus k is complex in $\alpha=A_0ke^{-bk}$.

Then

$$\rho = \frac{m^*\nu}{ne^2\hbar\nu}\exp\left[\frac{E_e+iE_i}{2k_BT}\right] \tag{16a}$$

$$\rho = \frac{\hbar k}{ne^2\hbar\nu}\exp\left[\frac{E_g}{2k_BT}\right]\exp\left[\frac{i\hbar\nu_g(k_1+ik_2)}{2k_BT}\right] \tag{16b}$$

$\sigma=\alpha n_1c/4\pi$ and $\sigma=(1/\rho)$ leads to oscillations in light absorption due to $\exp\left(i\hbar\nu_g k_i/2k_BT\right)$ factor. In the case of soft phonon mode the oscillatory behaviour is related with this $Q=2K_F$ modes becoming soft. In the present work the main aim is to explain light induced Peierls instability and Kohn anomaly. There are cases where under normal light or in dark Peierls distortion and Kohn anomaly do not take place but when intense incident light perturbs, Peierls instability appears because the mobile charge carriers drags lattice deformation or virtual phonon cloud.

3.3 Critical parameters for maximum conductivity

Thus $A=A_0\lambda e^{-b\lambda}$ and $A=A_0ke^{-bk}$ both follow electrical conductivity given by equation (14). Now let $V=K_BT$ and for maximum conductivity $\frac{d\sigma}{dT}=0$ leads to

$$-\frac{1}{2T}+\frac{E_g}{\left(2K_BT^2\right)}-i\left(\frac{E}{K_B}\right)^{\frac{1}{2}}\times\left(\frac{1}{2}\right)T^{-3/2}=0 \tag{17}$$

$E_g = E_c + E_i$ which gives $T_c = E_c/K_B = E_i^2/Ek_B$ implying $E = E_i^2/E_c$

T_c depends on ionic band gap.

For pressure, let $V=\gamma P^2$ (elastic energy is proportion to P^2). Also $\nu \sim P^{3/2}$ and $E_g = E_g^0 - \lambda P$. $(d\sigma/dP)=0$ condition for maximum conductivity is equivalent to

$$\frac{A}{2}\frac{1}{P^{1/2}}+AP^{1/2}\left(-\frac{\lambda}{2K_BT}\right)+i\left(\frac{E}{V}\right)^{1/2}P^{-3/2}=0 \tag{18}$$

The real part gives, $P_c = K_BT/\lambda$

where E_g to be real and not complex. When λ is large, P_c is small and when λ is small, P_c is high. For complex band gap, the condition becomes a quadratic equation given by

$$-\frac{1}{2}P+P^2\left(\frac{\lambda}{2K_BT}\right)\left(\frac{E}{\gamma}\right)^{\frac{1}{2}}\sin\frac{E_i}{2K_BT}=0 \tag{19}$$

Then

$$P_c=\frac{K_BT}{2\lambda}\pm\frac{K_BT}{\lambda}\sqrt{\frac{1}{4}-\left[4\left(\frac{\lambda}{2K_BT}\right)\left(\frac{E}{\gamma}\right)^{\frac{1}{2}}\sin\frac{E_i}{2K_BT}\right]} \tag{20}$$

Next for light or EM waves.

$V=\hbar\omega$ leads to $E=V=\hbar\omega_c$ or $\omega=E_c/\hbar$ for E_g to be real.

For complex band gap,

$$\omega_c=\left(\frac{E}{\hbar}\right)\cot\frac{E_i}{2K_BT} \tag{21}$$

This is one type of electron-phonon resonance.

For a particle in rectangular well [20]. $2E-V_0=2E^{1/2}\left(V_0-E\right)^{1/2}\times\cot\left[\left(2mE\right)^{1/2}L/\hbar\right]$

Now $E=1/2\,m\omega^2L^2$ or $L=(1/\omega)\left(\sqrt{2E/m}\right)$

Then $\hbar\omega=k_BT$ gives $E=E_0\cot\left[2E/k_BT\right]$ because for V_0 = 0, and $E_c=E\cot\left(2mE\right)^{1/2}L/\hbar$ after substituting L. This agrees with equation (21), when $E=E_i/4$.

Infrared band gaps like $E=E_i$, $E=E_i/2$ and $E_i = E_i/4$ are occasionally found where E_i is ionic band gap. E_i = 0.225 eV is the Peierls gap. Band gaps at 0.1125 and 0.0056 eVs are also found, because of electron-hole pairs (0.1125 eV) and biexciton generations (0.056 eV).

3.4 Transition temperature

Now we expand E in $b=i\left(\frac{E}{V}\right)^{\frac{1}{2}}\lambda$. Using $E=E_F+\left(\frac{dE}{dn}\right)_{E_F}\Delta n$ which gives

$$A=A_0e^{-i\left[\frac{\Delta n}{D(E_F)V}\right]^{\frac{1}{2}}(\lambda k)} \tag{22}$$

and taking $\lambda k=1$. Then

$$\sigma = i\frac{\left(ne^2\nu\hbar\right)e^{-\frac{E_g}{2K_BT}}\, e^{-i\left[\frac{\Delta n}{D(0)V}\right]^{\frac{1}{2}}}}{\left(2m^*E\right)^{\frac{1}{2}}\left(2m^*V\right)^{\frac{1}{2}}} \tag{23a}$$

E_F=0 (Fermi level is taken as zero).

So that D(E_F) = D(o).

Now the effective electron-electron interaction V is negative so that $V = -|V|$ leading to

$$|\sigma| = \left[\frac{\left(n_0e^2\nu\hbar\right)\exp\left(-\frac{E_g}{2k_BT}\right)\exp\left[\frac{\Delta n}{D(0)|V|}\right]^{\frac{1}{2}}}{\left(2m^*E\right)^{\frac{1}{2}}\left(2m^*V\right)^{\frac{1}{2}}}\right] \tag{23b}$$

Transition temperature through magnetic energy

Let us take an inductive response of a superconductor.

If L is the inductance depending on size, shape and geometry of the specimen, then magnetic energy is given by

$$E = \left(\frac{1}{2}\right)LI^2 = \left(\frac{1}{2}\right)|\sigma|^2\varepsilon^2A^2 = k_BT_c$$

where ε is the electric field.

then

$$T_c \cong \frac{\left(ne^2\nu\hbar\right)^2\left(\frac{1}{2}LA^2|\varepsilon|^2\right)\exp^2\left[\frac{\Delta n}{D(0)|V|}\right]^{\frac{1}{2}}\exp\left(-\frac{E_g}{k_BT}\right)}{\left(2m^*E\right)\left(2m^*V\right)K_B} \tag{24}$$

when the magnetic energy is equal to the available thermal energy ($k_BT_{c)}$ and T_c is the breaking temperature. In these case of photoconductivity [21] $Q = \eta W(1-R)/h\nu$ and $\Delta n = Q\Im_n$, where η is quantum efficiency,

$\Im_n$ is life time of charge carrier, W is watt of power incident, R is reflectivity and hν is photon energy.

Thus,

$$T_c \cong \frac{\left(ne^2\nu\hbar\right)^2\left(\frac{1}{2}LA^2|\varepsilon|^2\right)\times\exp\left(-\frac{E_g}{2k_BT}\right)\times\exp 2\left(\frac{\eta(1-R)\Im_n}{D(0)|V|h\nu}\right)^{1/2}}{\left(2m^*E\right)\left(2m^*V\right)K_B} \tag{25}$$

Thus as $\Im_n$, W and η increase, T_c increases. As |V|, hν and D(0) increase, T_c decreases.

For Δn arising from pressure, $E_g(P) = E_g^0 - \lambda P$ for Δn=-λPD(0)

$$T_c \cong \frac{\left(n_0 e^2 \nu \hbar\right)^2 \left(\frac{1}{2} L A^2 |\varepsilon|^2\right) \times \exp\left(-\frac{E_g}{k_B T}\right) \exp\left[-2\left(\frac{\lambda P}{|V|}\right)\right]^{\frac{1}{2}}}{\left(2m^* E\right)\left(2m^* V\right) K_B} \tag{26}$$

As P increases, T_c decreases as normally found in superconductors.

For temperature change [21],

$$E_g\left(T\right) = E_g^0 - \frac{\alpha T^2}{T+\beta} = E_g^0 - \left(\frac{\partial E}{\partial n}\right)_{E_E} \Delta n \tag{27}$$

leads to $\Delta n = -D\left(0\right)\alpha T^2 \big/ \left(T+\beta\right)$

where β is of the order of Debye temperature.

Then

$$T_c \cong \frac{\left(n e^2 \nu \hbar\right)^2 \left(\frac{1}{2} L A^2 |\varepsilon|^2\right) \times \exp\left(-\frac{E_g^0}{2 k_B T}\right) \times \exp\left[-2\left(\frac{\alpha T^2}{|V|(T+\beta)}\right)\right]^{\frac{1}{2}}}{\left(2m^* E\right)\left(2m^* V\right) K_B} \tag{28}$$

When α is small T_c is high.

In the above equations, E_g^0 is the band gap. E_g^0 is positive for a semiconductor. E_g^0 is Peierls gap for Peierls semiconductor. E_g^0=0 for metals and two dimensional conductors at low temperatures, E_g^0 is negative for semimetals and E_g^0 is BCS gap for superconductors. Thus the above equations apply generally to conducting solids of all types.

3.5 Power dissipation and the breaking temperature

For $\alpha = \alpha_0 k e^{-bk}$ function as observed in infrared spectra of some organic and metal-organic charge transfer complexes, the spectral function is $A = A_0 b \big/ \left(b^2 + \lambda^2\right)$ where λ is deformation. Power dissipation is related with absorption as follows. Power $P=I^2R=|\sigma|\varepsilon^2V'$ where E is electric field, σ is conductivity and V' is volume.

$P = \Gamma k_B T_c$ also where Γ is a constant.

Then

$$\sigma = \left(\frac{n_1 c}{4\pi}\right) A_0 \frac{b}{b^2+\lambda^2} \tag{29}$$

Substituting A_0 and b given by equation15a and 15b, simplifying and using T=E-V,

$$T_c \cong -\frac{\left(ne^2\nu\hbar\right)|\varepsilon|^2 V'}{\Gamma K_B\left(2m^*T\right)} \tag{30}$$

and some equation as (30)

For $A = A_0\lambda e^{-b\lambda}$ the spectral function is $A = A_0\, b\big/\left(b^2+k^2\right)$ exactly similar analysis using 13a and 13b leads to

$$\Gamma k_B T_c \cong \left(\frac{n_1 c}{4\pi}\right) A_0 \frac{b}{b^2+k^2}\left|\varepsilon^2\right| V' \tag{31}$$

As m^*-the effective mass is less, T_c is high. When kinetic energy (T) is less, T_c is high. This shows CDWs that move very slowly with very less kinetic energy and Frohlich superconductor has T_c higher than BCS superconductors.

3.6 Pressure and temperature dependence of resistivity or conductivity

The pressure dependence of resistivity of some inclusion compounds of iodine and benzidine-TCNQ are given by $\rho(P) = \rho_0(P)\exp(-bP)$; the spectral function is given by

$\sigma = \left(1\big/A_0 b\right)\left(b^2+x^2\right)$ where x is deformation.

$\sigma = ne^2\nu\lambda\big/m^*\nu = ne^2\nu\lambda^2\big/\hbar$ taking k=1/λ. Then

$$\sigma = \frac{ne^2\nu}{\hbar}\frac{2}{C}(E-T) \tag{32}$$

using $(1/2)C\,\lambda^2 = E-T$. Comparing constant and variable terms, A_0 and b are found.

Substitution back in formula for conductivity leads to

$$\sigma = -i\left(\frac{2ne^2\nu}{\hbar c}\right)\frac{\sqrt{ET}}{xP}\exp\left[+i\left(\frac{E}{T}\right)^{\frac{1}{2}} xP\right] \tag{33}$$

Power P' is proportional to $|\sigma^2|$ for inductive response $\frac{1}{2}LI^2 = k_B T_c \infty |\sigma|^2$ leads to

$$T_c = \frac{1}{k_B}\frac{1}{2}LA^2|\varepsilon|^2\left(\frac{2n_0e^2\nu}{\hbar c}\right)^2\left[\exp-\frac{\left(E_g^0-\lambda P\right)}{k_B T}\right]\left(\frac{ET}{W^2}\right) \tag{34}$$

The factor

$\left[\exp\left[-i\left(E/T\right)\right]^{1/2} W\right]$ where $\left(W = xP\right)$ remains imaginary and cancels out while taking modulus $|\sigma|$.

Next power dissipation $P = I^2R = \sigma|E|^2 V' = \Gamma\, k_B T_c \propto |\sigma|$ and leads to

$$T_c = \left(\frac{|\varepsilon|^2 V'}{\Gamma K_B}\right)\left(\frac{2ne^2\nu}{\hbar c}\right)\frac{\sqrt{ET}}{W}\left[\exp - i\left(\frac{E}{T}\right)^{\frac{1}{2}} W\right]\times\exp\left(-\frac{E_g^0 - \lambda P}{2K_B T}\right) \tag{35}$$

Note T is negative when effective mass is negative.

Now $\rho = A'P\exp(-b'P)$ where P is momentum.

$A_0' = A_0/\Im A'$ and $b' = b/\Im A'$ P is pressure, $\Im$ is relaxation time and $P = \left(dP/dt\right)A' = p/\Im A'$ where A' is area under compression. Then

$$\rho = i\left(\frac{\hbar c}{2ne^2\nu}\right)\frac{xP}{\sqrt{ET}}\exp - i\left(\frac{E}{T}\right)^{\frac{1}{2}} xP \tag{36}$$

So that

$$\rho = i\left(\frac{\hbar C}{2ne^2\nu}\right)\frac{x}{\sqrt{E/2m^*}}\,\mathrm{e}^{-i\left(2m^*E\right)^{\frac{1}{2}}}\left(x\right) \tag{37}$$

If m* is positive, the resistivity oscillates with x. If m* is negative, resistivity exponentially falls to zero.

The temperature dependence of the conductivity (σ) is given by $\sigma(T) = A_0 T e^{-bT}$ as found experimentally in cadmium oxalate, $\rho = \left(b^2 + S^2\right)/A_0 b$ this should be compared with $\rho = 2m^*(E - V)/ne^2\nu\hbar$ to determine A_0 and b. S is entropy. Exactly similar analysis as carried out in light-induced Peierls instability leads to

$$\sigma = i\frac{(ne^2\nu\hbar)(ST)\exp - i\left(\frac{E}{V}\right)^{\frac{1}{2}} ST}{\left(2m^*V\right)^{\frac{1}{2}}\left(2m^*E\right)^{\frac{1}{2}}} \tag{38a}$$

$$\sigma = \frac{i(ne^2\nu\hbar)U_0\exp\left(\frac{\Delta n}{D(0)|V|}\right)^{\frac{1}{2}} U_0}{\left(2m^*V\right)^{\frac{1}{2}}\left(2m^*E\right)^{\frac{1}{2}}} \tag{38b}$$

where U_0 = ST is the internal energy. This leads to $P = \Gamma K_b T_c = I^2 R\infty|\sigma|$ and

$$T_c = \left(\frac{|\varepsilon|^2 V'}{\Gamma K_B}\right)\frac{n_0 e^2\nu\hbar U_0\exp\left(\frac{\Delta n}{D(0)|V|}\right)^{\frac{1}{2}} U_0}{\left(2m^*V\right)^{\frac{1}{2}}\left(2m^*E\right)^{\frac{1}{2}}} \tag{39}$$

From magnetic energy $\left(\frac{1}{2}\right)LI^2 = k_B T_c \infty |\sigma|^2$ gives $\left(\frac{1}{2}\right)\varepsilon |E|^2 A^2$

$$T_c \cong \frac{1}{K_B}\left(\frac{1}{2}L|\varepsilon|^2 A^2\right)\frac{(ne^2\nu\hbar)^2 U_0^2 \exp 2\left(\frac{\Delta n}{D(0)(V)}\right)^{\frac{1}{2}} U_0}{(2m^*V)(2m^*E)} \tag{40}$$

For $P = I^2 R = \Gamma K_b T_c \infty |\sigma|$

$$T_c = \frac{\left(\frac{n_1 c}{4\pi}\right) A_0 \left(\frac{b}{b^2+\lambda^2}\right)|\varepsilon|^2 V'}{\Gamma k_B} \tag{41}$$

Substitution of A$_0$ and b, simplifying and using V=E-T gives

$$T_c \cong -\frac{(ne^2\nu\hbar)|\varepsilon|^2 V'}{\Gamma k_B (2m^*V)^{\frac{1}{2}}(2m^*T)^{\frac{1}{2}} V} \tag{42}$$

For temperature dependence, $\sigma = A_0 b \big/ \left(b^2 + S^2\right)$ where S is entropy. The substitution of A$_0$ and b leads to the equation which is same as equation (30).

3.7 Gaussian absorption and transition temperature

The Gaussian absorption function [23] is given by

$$\alpha = A_0 \exp\left[-\frac{\left(\lambda-\lambda_0\right)^2}{2M_2}\right] \tag{43a}$$

$$\dot{\alpha} = \dot{A}_0' \exp\left[-\frac{\left(k-k_0\right)_2}{2\dot{M}_2'}\right] \tag{43b}$$

where A$_0$is maximum absorption, λ is wave length, λ$_0$ is central value of λ and M$_2$ is the second moment of the Gaussian distribution (20). The Fourier transform of a Gaussian function is also a Gaussian function. A', k$_0$ and M_2' are the same Gaussian parameters as A$_0$, λ$_0$ and M$_2$.

Now

$$\ln\rho = \frac{2m^*}{ne^2\nu\hbar} + \ln(E-V) \tag{44a}$$

and for Gaussian

$$\ln\rho = \ln\left(\frac{4\pi}{n_1 c\dot{\alpha}}\right) + \ln\frac{\left(k-\dot{k}_0\right)^2}{2M_2} \tag{44b}$$

Comparing constant and variable terms,

$$2M_2 = \frac{(k-k_0)^2}{\ln(E-V)} = \frac{(k-k_0)^2}{\ln\left(p^2/2m^*\right)} \tag{45}$$

As m* increases, $2\dot{M}_2$ increases, i.e. the width of the Gaussian function increases as the effective Frohlich mass increases. Also the amplitude decreases i.e. less pronounced Gaussian bands are better for Frohlich super conduction. As an approximation

$$\alpha = \alpha_0 \left[1 + \frac{(k-k_0)^2}{2M_2}\right] \tag{46}$$

Which is a Cauchy distribution. For $2\dot{M}_2 >> (k-k_0)^2$.This is a Cauchy distribution. Now since

$$\frac{2m^* E}{ne^2 \nu \hbar} = \frac{4\pi}{n_1 c \alpha_0} \tag{47a}$$

and $-\frac{2m^* V}{ne^2 \nu \hbar} \cong \frac{4\pi}{n_1 c \alpha_0} \frac{(k-k_0)^2}{2\dot{M}_2}$ (47b)

by expanding 1/∝.

$$2M_2 \cong -\frac{E}{V}(k-k_0)^2 \tag{48}$$

which in turns gives

$\alpha = \alpha_0 \exp\left[-(k-k_0)^2/2\dot{M}_2\right]$ $\alpha = \alpha_0 \exp(V/E) = \alpha_0 \exp(-|V|/E)$ since V= - | V |

$$\alpha = \alpha_0 \exp\left[-\left(\frac{|V|}{E_F + \left.\frac{\partial E}{\partial n}\right|_{E_F} \Delta n}\right)\right] \tag{49}$$

Taking D(E$_F$) = D(0), $\alpha = \alpha_0 e\,\mathrm{xp}\left[-|V|D(0)/\Delta n\right]$where the Fermi level (E$_F$) is taken as zero. $\sigma = (n_1 c/4\pi) A_0 \exp\left[-|V|D(0)/\Delta n\right]$and as | V | and D(0) increase, σ decreases.

Now $K_B T_c = (1/2) LA^2 |E|^2 \sigma^2$, where L is inductance,

then

$$T_c \cong \frac{1}{K_B}\left(\frac{1}{2} LA^2 |\varepsilon|^2\right)\left(\frac{n_1 c}{4\pi}\right)^2 \dot{A}_0^2 \exp-\left[2\left(\frac{|V|D(0)}{\Delta n}\right)\right] \tag{50}$$

As | V | and D(0) decrease T$_c$ increases.

and Γk$_B$T$_c$ = I^{2}R=| σ | | E^2 | V$'$ leads to

$$T_c \cong \left(\frac{|\varepsilon|^2 V'}{\Gamma k_B} \right) \left(\frac{n_1 c}{4\pi} \right) A_0 \exp\left[-\frac{|V| D(0)}{\Delta n} \right] \qquad (51)$$

IV. CONCLUSION

Seven polyiodide chains complexes shows $A(\lambda)=A_0\ \lambda^{-b\lambda}$ relation in UV-visible which shows Cauchy distribution in momentum. $A(k)=A_0\ ke^{-b\lambda}$ function is found in TTF-TCNQ and TMTSF-DDQ and two CT complexes of Ni (N-CH_3-Salim)$_2$ which is associated with dynamic anomaly or light induced Kohn anomaly. Oscillations are related with optically detected charge density waves in other materials. It is possible to get an equation for transition temperature when the thermal energy compensates magnetic energy or power loss obtained in the Frohlich current.

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