Theory of pseudogaps in charge density waves in application to photo electron or tunneling spectroscopy.

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Abstract

For a one-dimensional electron-phonon system we consider the photon absorption involving electronic excitations within the pseudogap energy range. In the framework of the adiabatic approximation for the electron - phonon interactions these processes are described by nonlinear configurations of an instanton type. We calculate the subgap absorption as it can be observed by means of photo electron or tunneling spectroscopies. In details we consider systems with gapless modes: 1D semiconductors with acoustic phonons and incommensurate charge density waves. We find that below the free particle edge the pseudogap starts with the exponential decrease of transition rates changing to a power law deeply within the pseudogap, near the absolute edge.
I. PSEUDOGAP, SOLITONS, INSTANTONS.

This article is devoted to theory of pseudogaps (PGs) in applications to Photo Electron Spectrography (PES). We shall study influence of quantum lattice fluctuations upon electronic transitions in the subgap region for one-dimensional (1D) systems with gapless phonons. We will show that sound branches of phonon spectra change drastically transition rates making them much more pronounced deeply within the PG. We shall consider generic 1D semiconductors with acoustic e-ph coupling and Incommensurate Charge Density Waves (ICDWs) which possess the gapless collective phase mode.

Details and illustrations can be found in [3]. Low symmetry systems with gapful spectra have been addressed by the authors earlier [4] and we refer to this article for a more comprehensive review and references.

The PG concept introduced in [5] refers today to various systems where a gap in their bare electronic spectra is partly filled showing subgap tails. Even for pure systems and at zero temperature there may be a rather smeared edge $E^0_g$ while the spectrum extends deeply inwards the gap till some absolute edge $E_g < E^0_g$ which may be even zero (no true gap at all). A most general reason is that stationary excitations (eigenstates of the total e-ph system) are the self-trapped states, polarons or solitons [6] which energies, $W_p$ or $W_s$, are below the ones of free electrons thus forming $E_g = W_p, W_s$. Nonstationary states filling the PG range $E^0_g > E > E_g$ can be observed only via instantaneous measurements like optics, PES or tunneling. Particularly near $E^0_g$ the states resemble free electrons in the field of uncorrelated quantum fluctuations of the lattice [6]; here the self-trapping has not enough time to be developed. But approaching the exact threshold $E_g$, the excitations evolve towards eigenstates which are self-trapped e-ph complexes. The PGs must be common in 1D semiconductors just because of favorable conditions for self-trapping [7]. The PG is especially pronounced when the bare gap is opened spontaneously as a symmetry breaking effect. In quasi-1D conductors it is known as the Peierls-Fröhlich instability leading to the CDW formation. Here the PGs were addressed experimentally by means of optics [8], PES [9] and by the new methodics of the coherent interlayer tunneling [10].

Detailed theories of the subgap absorption in optics have been developed already for systems with low symmetries (nondegenerate, like semiconductors with gapful phonons, or discretely degenerate like the dimerized Peierls state): for a general type of polaronic semi-
conductors [11] with an emphasis to long range Coulomb effects and for the one dimensional Peierls system with an emphasis to solitonic processes [12]. Recently the authors [4] extended the theory of pseudogaps to single electronic spectra in application to the PES and, particularly intriguing, to the ARPES (momentum resolved PES) probes. But properties of ICDWs are further complicated by appearance of the gapless collective mode which bring drastic changes. The case of acoustic polarons in 1D semiconductors belongs to the same class.

The specifics of 1D systems with continuous degeneracy (with respect to the phase for the ICDW, to displacements for usual crystals) is that even single electronic processes can create topologically nontrivial excitations, the solitons. Thus for the ICDW a single electron or hole with the energy near the gap edges $\pm \Delta_0$ spontaneously evolves to the nearly amplitude soliton - AS whilst the original electron is trapped at the local level near the gap center [6]. The energy $\approx 0.3\Delta_0$ is released, at first sight within a time $\omega_{ph}^{-1} \sim 10^{-12}s$. We will see that actually there is also a long scale adaptation process which determines transition probabilities. Similarly, the usual acoustic polaron in a 1D semiconductors is characterized by the electronic density $\rho$ selflocalized within the potential well $\sim \partial \varphi / \partial x \sim \rho$, hence a finite increment $\varphi(+\infty) - \varphi(-\infty) \neq 0$ of the lattice displacements $\varphi(x)$ over the length $x$ which is the signature of topologically nontrivial solitons.

II. INSTANTON APPROACH TO PSEUDOGAP

We shall use the adiabatic approximation valid when changes of electronic energies are much bigger than relevant phonon frequencies. Electrons are moving in the slowly varying potential, e.g. $\text{Re}\{\Delta(x,t) \exp[i2k_F x]\}$ for the ICDW. So at any instance $t$ their energies $E(t)$ and wave functions $\psi(x,t)$ are defined as eigenstates for the instantaneous lattice configuration and they depend on the time $t$ only parametrically. The PES absorption rate $I(\Omega)$ for the light frequency $\Omega$ can be written as the functional integral

$$I(\Omega) \propto \int_0^\infty dT \int D[\Delta(x,t)] \psi_0(0,T)\psi_0^+(0,0) \exp(-S)$$

were $\psi_0$ is the wave function of the particle (for the PES it is actually a hole) added and extracted in moments 0 and $T$ at the fluctuational intragap level $E_0$. The time $t,T$ is already chosen along the imaginary axis where the saddle points of this integral are commonly
believed to be found (see [4, 11] for references). The Euclidean action

\[ S[\Delta(x,t),T] = (\int_{-\infty}^{0} + \int_{T}^{\infty}) dt L_0 + \int_{0}^{T} dt (L_1 - \Omega) \]

is determined by Lagrangians \( L_j \) where the labels \( j = 0,1 \) correspond to ground states for \( 2M \) (the bare number) and \( 2M \pm 1 \) electrons in the potential \( \Delta(x,t) \). For calculations of subgap processes only the lowest singly filled localized state is relevant which energy \( E_0 \) is split off inside the gap, hence \( L_1 = L_0 + E_0 \). The main contribution comes from saddle points of \( S \), the instantons, which are extremas with respect to both the function \( \Delta(x,t) \) and the time \( T \), the last condition yielding \( E_0(T) = \Omega \).

### III. CREATION OF SPIN SOLITONS IN INCOMMENSURATE CDWS.

For the ICDW the order parameter is the complex field \( \Delta = |\Delta(x,t)| \exp[i\varphi(x,t)] \) acting upon electrons by mixing states near the Fermi momenta points \( \pm k_F \). The Lagrangians \( L_j \) consist of the bare kinetic \( \sim |\partial_t \Delta|^2 \) and potential \( \sim |\Delta|^2 \) lattice energies and of the sum over the filled electron levels:

\[ L_j = \frac{2}{\pi v_F} \int dx |\partial_t \Delta|^2 / \omega_0^2 + V_j[\Delta(x,t)] \]

where \( v_F \) is the Fermi velocity in the metallic state and \( \omega_0 \ll \Delta_0 \) is the amplitude mode frequency in the CDW state. The stationary state with an odd number of particles, the minimum of \( V_1 \), is the amplitude soliton (AS) \( \Delta \Rightarrow -\Delta \) with the midgap state \( E_0 = 0 \) occupied by the singe electron. The evolution of the free electron to the AS can be fortunately described by the known exact solution for intermediate configurations characterized by the singly occupied intragap state \( \nu = 0,1 \) corresponds to labels \( j = 0,1 \). The term \( V_0(\theta) \) increases monotonically from \( V_0(0) = 0 \) for the \( 2M \) ground state (GS) to \( V_0(\pi) = 2\Delta_0 \) for the \( 2M + 2 \) state with two free holes. The term \( V_1(\theta) = V_1(\pi - \theta) \) is symmetric describing both the particle upon the \( 2M \) GS and the hole upon the \( 2M + 2 \) GS. Apparently \( V_1(0) = V_1(\pi) = \Delta_0 \) while the minimum is reached at \( \theta = \pi/2 \) that is for the purely AS: \( \min V(\theta) = V_1(\pi/2) = W_s < \Delta_0 \) where \( W_s = 2/\pi \Delta_0 \) is the AS energy. To create a nearly AS with \( \theta = 90^\circ \), the light with \( \Omega \approx W_s \) is absorbed
by the quantum fluctuation with $E_0(\theta) = W_s$ which is close to the chordus soliton with the angle $\theta \approx 50^\circ$.

As the topologically nontrivial object, the AS cannot be created in a pure form: adaptational deformations must appear to compensate for the topological charge. These deformations are developing over long space-time scales and they can be described in terms of the gapless mode, the phase $\varphi$, alone. Hence allowing for the time evolution of the chiral angle $\theta \rightarrow \theta(t)$ within the core, we should also unhinder the field $\varphi \rightarrow \varphi(x,t)$ at all $x$ and $t$. Starting from $x \rightarrow -\infty$ and returning to $x \rightarrow \infty$ the system follows closely the circle $|\Delta| = \Delta_0$ changing almost entirely by phase. Approaching the soliton core the phase matches approximately the angles $\pm \theta$ which delimit the chordus part of the trajectory. The whole trajectory is closed which allows for the finite action $S$. The chordus angle $2\theta(t)$ evolves in time from $\theta(\pm \infty) = 0$ to $\theta_m$ in the middle of the $T$ interval. For $T \rightarrow \infty$, that is near the stationary state of the AS, $\theta_m \rightarrow \pi/2$. Actually this value is preserved during most of the $T$ interval so that changes between $\theta = 0$ and $\theta = \pi/2$ are concentrated within finite ranges $\tau \sim \xi_0/u \ll T$ near the termination points. From large scales we view only a jump $\varphi(x,t) \approx \theta(t)\text{sgn}(x)$ with $\theta(t) \approx \pi/2\Theta(T-t)$ for a well developed AS. Since the configuration stays close to the AS during the time $T$, the main core contribution to the action is

$$S_{\text{core}} = (W_s - \Omega)T + \delta S_{\text{core}}$$

where the first correction $\delta S_{\text{core}}^0 = \text{cnst}$ comes form regions around moments $0, T$ independently. The significant $T$ dependent contribution $\delta S(T)$ comes from interference of regions $0$ and $T$ which for the ICDW communicate via the gapless phase mode. Its effect can be easily extracted if we generalize the scheme suggested earlier for static solitons at presence of interchain coupling $13$. The action for the phase mode is

$$S_{\text{snd}}[\varphi(x,t),\theta(t)] = \frac{v_F}{4\pi} \int \int dxdt \left( (\partial_t \varphi/u)^2 + (\partial_x \varphi)^2 \right)$$

where $u$ is the phase velocity. The chordus soliton forming around $x_s = 0$ enforces the discontinuity $\varphi(t,\pm 0) = \mp \theta(t)$. Integrating out $\varphi(x,t)$ from $\exp\{-S_{\text{snd}}[\varphi,\theta]\}$ we arrive for $\theta(t)$ at the typical action for the problem of quantum dissipation $14$

$$S_{\text{snd}}[\theta] \approx -\frac{v_F/|u|}{2\pi^2} \int \int dt_{1,2} \dot{\theta}(t_1) \ln |(t_1 - t_2)| \dot{\theta}(t_2)$$
that is $S \sim \sum |\omega||\theta_\omega|^2$. The dissipation comes from emission of phase phonons while forming the long range tail in the course of the chordus soliton development. This action, together with $V_j$, can be used to prove the above statements on the time evolution of the ChS core.

Remember now that $\partial_t \theta$ is peaked within narrow regions $\sim \xi_0/u$ around moments $t = 0$ and $t = T$ and close to zero otherwise. Then

$$S_{\text{snd}} \approx (v_F/4u) \ln(uT/\xi_0)$$

The picture is clear in the space-time domain. The AS creates the $\pi-$ discontinuity along its world line: $(0 < t < T, x = 0)$. To be topologically allowed, that is to have a finite action, the line must terminate with half integer vortices located at $(0, 0)$ and $(0, T)$ which circulation provides the jump $\delta \varphi = \pi$ along the interval compensating for the sign change of the amplitude ($\Delta \Rightarrow -\Delta$ combined with $\varphi \Rightarrow \varphi + \pi$ leaves the order parameter $\Delta \exp(i\varphi)$ invariant, see [15] for discussion of ”combined topological defects”). Then the standard energy of vortices for (1) leads identically to the action (2). Contrary to usual $2\pi-$ vortices, the connecting line is the physical singularity which tension gives $S_{\text{core}}$.

Minimizing $S_{\text{tot}} = S_{\text{core}} + S_{\text{snd}}$ with respect to $T$, we obtain near the AS edge $\Omega \geq W_s$ the power law

$$I(\Omega) \propto \left(\frac{\Omega - W_s}{W_s}\right)^\beta, \quad \beta = \frac{v_F}{4u}$$

which is much more pronounced than the nearly exponential law [4] for gapful cases: $I \sim \exp\{-\delta \Omega \ln(\delta \Omega)\}$.

Behavior near the free edge $\Omega \approx \Delta_0$ is dominated by small fluctuations $\eta$ of the gap amplitude $|\Delta| = \Delta_0 + \eta$ and of the Fermi level $\delta E_F = \varphi'/v_F/2$ via the phase gradient $\varphi' = \partial_x \varphi$. We shall analyze it in a frame of a generic problem of the combined (gapful and acoustic) polaron where the simpler single particle formulation allows for a more detailed analysis.

IV. 1D SEMICONDUCTORS: FROM POLARONS TO QUANTUM NOISE.

Consider electron (hole) states in a 1D dielectric near the edge of a conducting (valence) band. We shall take into account the gapful phonon mode $\eta$ with the coupling $g_0$ and the sound mode (for which we shall keep the ”phase” notation $\varphi(x, t)$) with the velocity $u$ and the coupling $g_s$. In generic semiconductors the sound mode is always present as the acoustic
phonon while the gapful one can be present as an additional degree of freedom. In CDWs
the gapful mode is always present as the amplitude fluctuation $|\Delta| = \Delta_0 + \eta$ while the sound
mode appears in the ICDWs as the phase $\Delta = |\Delta| \exp[i\varphi]$.

Within the adiabatic approximation the action $S$ has the form

$$\int dx \int dt \left[ \frac{1}{2m} |\Psi'|^2 - \Omega |\Psi|^2 \right] + (g_s \varphi' + g_0 \eta) |\Psi|^2 \right] +$$

$$\int dx dt \left[ \frac{K_s}{2} (\dot{\varphi}^2 / u^2 + \varphi^2) + \frac{K_0}{2} (\dot{\eta}^2 / \omega_0^2 + \eta^2) \right] .$$

(For the PES problem, the electron wave function $\psi = psi(x, t)$ is not zero only at $0 < t < T$.
Thus for the ICDW case we have $m = \Delta_0 / v_F$, $g_s = g_s / 2$, $K_s = v_F / 2\pi$, $K_0 = 4 / \pi v_F,$
$2^{3/2} u / v_F = \omega_0 / \Delta_0$ and $\Omega$ is counted with respect to $\Delta_0$. The stationary state, the time
independent extremum of (4), corresponds to the selftrapped complex, the polaron \[7\]. Here
it is composed equally by both $\eta$ and $\varphi'$ which contribute additively to the coupling $\lambda =$
$\lambda_s + \lambda_0 = g_s^2 / K_s + g_0^2 / K_0$. The polaronic length scale $l$ for $\eta \sim \varphi' \sim |\Psi|^2 \equiv \rho_p(x)$ is $l = 2 / m \lambda$
and the total energy is $W_p = -m \lambda^2 / 24$. The conditions $|W_p| \gg \omega_0$ and $\lambda \gg u$ define the
adiabatic approximation. For the CDW case $\lambda_s = v_F \pi / 2$ and $\lambda_0 = v_F \pi / 4$ hence $\lambda \sim v_F$
and we would arrive at $|W_p| \sim \Delta_0$ and $l \sim \xi_0 = v_F / \Delta_0$ which are the microscopic scales
where the single electronic model may be used only qualitatively. The full scale approach
for nearly stationary states has been considered above, but the upper PG region near the
free edge $\Delta_0$ will be described by the model [4] even quantitatively.

We can integrate out the fields $\varphi$ and $\eta$ at all $x,t$ to obtain the action $S\{\Psi; T\}$ in terms
of $\Psi$ alone which is defined now only at the interval $(0,T)$:

$$\int dx dt \left( \frac{1}{2m} |\partial_x \Psi|^2 - \Omega |\Psi|^2 \right) - \frac{1}{2} \int dt_1 \int \int dx_{1,2} \{U_s(\delta_{1,2}) \rho'(x_1, t_1) \rho'(x_2, t_2) \} + U_0(\delta_{1,2}) \rho(x_1, t_1) \rho(x_2, t_2)$$

where $\delta_{1,2} = (x_1 - x_2, t_1 - t_2)$ and

$$U_s = \frac{\lambda_s u}{2\pi} \ln \sqrt{x^2 + t^2 u^2}, \quad U_0 = \frac{1}{2} \lambda_0 \omega_0 \exp[-\omega_0 |t|] \delta(x)$$

An equivalent form for $S\{\Psi; T\}$, suitable at large $T$, is obtained via integrating by parts:

$$\int dx \int dt \left( \frac{1}{2m} |\Psi'|^2 - \Omega \rho - \frac{\lambda}{2} \rho^2 \right) + \frac{1}{2} \int dt_1 \int dx_{1,2} \rho(1) U(\delta_{1,2}) \rho(2)$$
where \( U(x,t) = u^{-2}U_s + \omega_0^{-2}U_0 \).

The absorption near the absolute edge \( \Omega \approx W_p \) is determined by the long time processes when the lattice configuration is almost statically self-consistent with electrons. The first term in (7) is nothing but the action \( S_{st} \) of the static polaron which extremum at given \( T \) is \( S_{st} \approx -T\delta\Omega \), \( \delta\Omega = \Omega - W_p \). The second term in (7) \( S_{tr} \) collects contributions only from short transient processes near \( t = 0, T \) which are seen as \( \partial_t \rho(x,t) \approx \rho_p(x)[\delta(t) - \delta(t - T)] \) where \( \rho_p \) is the density for the static polaron solution. We obtain

\[
S_{tr} \approx \int \int dx_1 dx_2 \rho_p(x_1)\rho_p(x_2)U(x_1 - x_2, T)
= \frac{\lambda_s}{2\pi u} \ln \frac{uT}{l} + C_0 \frac{\lambda_0/l}{\omega_0} \exp[-\omega_0 T] + \text{cnst}
\]

with \( C_0 \sim 1 \). We see the dominant contribution of the sound mode which grows logarithmically in \( T \) while the part of the gapful mode decays exponentially. If the sound mode is present at all, then the extrema over \( T \) is

\[
T \approx \frac{\lambda_s}{2\pi u} \frac{1}{\delta\Omega} ; \quad S \approx \frac{\lambda_s}{2\pi u} \ln \frac{C_s|W_p|}{\delta\Omega} , \quad C_s \approx 0.9
\]

We find that near the absolute edge \( \Omega \approx W_p \) the absorption is dominated by the power law \( I \sim |\delta\Omega/W_p|^\alpha \), with a big index \( \alpha = \lambda_s/(2\pi u) \). For parameters of the ICDW we obtain \( \alpha = v_F/4u = \beta \) in full accordance with the exact treatment (3).

Only in absence of sound modes \( \lambda_s = 0 \) the gapful contribution can determine the absolute edge. Then the minimization over \( T \) of \( S = S_{core} + \delta S_{gap} \) would lead qualitatively to the result of (4):

\[
I \sim \exp \left( \text{cnst} \frac{\Omega - W_p}{\omega_0} \ln \frac{W_s}{(\Omega - W_s)} \right)
\]

for the intensity near the absolute edge.

The opposite regime near the free edge \( \Omega \approx 0 \) (\( \Omega \Rightarrow \Omega - \Delta_0 \) for the ICDW) is dominated by fast processes of quantum fluctuations. Their characteristic time \( T = T(\Omega) \) is short in compare to the relevant phonon frequency: \( T \ll \omega_0, u/L \), where \( L = L(\Omega) \) is the characteristic localization length for the fluctuational electronic level at \( E_0 = \Omega \). Neglecting time variations within the short interval \( (0, T) \), we can estimate the action (5), term by term, as

\[
S \approx \frac{C_1 T}{mL^2} - \Omega T - C_2 \lambda_s u \left( \frac{T}{L} \right)^2 - C_3 \lambda_0 \omega_0 \frac{T^2}{L}
\]
with $C_i \sim 1$. Its extremum over both $L$ and $T$ yields

$$S \sim \frac{|\Omega|^{3/2}/m^{1/2}}{\max \{|m\Omega|^{1/2}u\lambda_s; \omega_0\lambda_0\}}$$  \hspace{1cm} (8)

Then $I \sim \exp(-S)$ interpolates between the closest $S \sim |\Omega|^{3/2}$ and the more distant $S \sim |\Omega|$ vicinities of the free electronic edge. For the purely acoustic case $\lambda_0 = 0$ a variational estimation for the numerical coefficient as $C_1 \approx 1/6, C_2 \approx 0.06$ gives

$$I \sim \exp[-\text{cst}|\Omega|/n\mu\lambda_s], \text{ cconst } \approx 2.8$$  \hspace{1cm} (9)

V. CONCLUSIONS.

We conclude that the subgap absorption in systems with gapless phonons is dominated by formation of long space-time tails of relaxation. It concerns both the acoustic polarons in 1D semiconductors and solitons in ICDWs. Near the free edge the simple exponential, Urbach type, law (9) appears competing with stretched exponential ones typical for tails from optimal fluctuations, see (8). The deeper part of the PG is dominated by the power law (3) (with the big dependable index) singularity near the absolute edge.

Our results have been derived for single electronic transitions: PES and tunneling. They can also be applied to intergap (particle-hole) optical transitions as long as semiconductors are concerned. For the ICDW results are applied to the free edge vicinity. But the edge at $2E_s$ will disappear in favor of optically active gapless phase mode.

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