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PSEUDOGAPS IN INCOMMENSURATE CHARGE DENSITY WAVES AND ONE-DIMENSIONAL SEMICONDUCTORS

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We consider pseudogap effects for electrons interacting with gapless modes. We study generic $1D$ semiconductors with acoustic phonons and incommensurate charge density waves. We calculate the subgap absorption as it can be observed by means of photoelectron or tunneling spectroscopy. Within the formalism of functional integration and adiabatic approximation, the probabilities are described by nonlinear configurations of an instanton type. Particularities of both cases are determined by the topological nature of stationary excited states (acoustic polarons or amplitude solitons) and by the presence of gapless phonons that change the usual dynamics to the quantum dissipation regime. Below the free-particle edge, the pseudogap starts with an exponential (stretched exponential for gapful phonons) decrease of the transition rates. Deeply within the pseudogap, they are dominated by a power law, in contrast to a nearly exponential law for gapful modes.

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1. INTRODUCTION: PSEUDOGAPS IN 1*D* SYSTEMS

This paper is devoted to the theory of pseudogaps in electronic spectra in application to photoelectron spectroscopy (PES). We study the influence of quantum lattice fluctuations on electronic transitions in the subgap region for one-dimensional ($1D$) systems with gapless phonons. Low-symmetry systems with gapful spectra were recently addressed by the authors [1], and we refer to this paper for a more comprehensive review and references. Here, we show that sound branches of phonon spectra drastically change the transition rates making them much more pronounced deeply within the pseudogap. We consider two types of systems: generic $1D$ semiconductors with acoustic electron–photon (*e*–*ph*) coupling (conducting polymers, quantum wires, and nanotubes) and incommensurate charge density waves (CDWs) [2], which possess a gapless collective phase mode.

The pseudogap concept [3] refers to various systems where the gap in their bare electronic spectra is partly filled and subgap tails occur. Even for pure systems and at temperature $T = 0$, there can be a rather smeared edge E_g^0, while the spectrum extends deeply inward the gap until some absolute edge E_g, which can be even zero (no true gap at all). A most general reason is that stationary excitations (eigenstates of the total *e*–*ph* system) are self-trapped states, polarons or solitons, whose energies W_p and W_s are below the free electron ones, thus forming the absolute edge at $E_g < E_g^0$. Nonstationary states filling the pseudogap range $E_g^0 > E > E_g$ can be observed only via instantaneous measurements like optics, PES, or tunneling. Particularly near E_g^0, the states resemble free electrons in the field of uncorrelated quantum fluctuations of the lattice [4]; here, the self-trapping does not have enough time to develop. But approaching the exact threshold E_g, the excitations evolve towards eigenstates, which are self-trapped *e*–*ph* complexes. The pseudogaps must be common in $1D$ semiconductors just because of favorable conditions for self-trapping [5]. The pseudogap is especially pronounced when the bare gap is opened spontaneously as a symmetry breaking effect. In quasi-$1D$ conductors, this symmetry break-

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ing is known as the Peierls–Fröhlich instability leading to the CDW formation. Here, the picture of the pseudogap was first suggested theoretically [3] (we also recall [6] and another model [7]) in relation to the absence of a long-range order in $1D$ CDWs at a finite temperature. In this approach, the smearing of the mean-field electronic gap $2\Delta_0$ corresponds to the disappearance of the true Peierls–Fröhlich transition in favor of a smooth crossover. The pseudogap shape was related to, and derived from, the temperature-dependent finite correlation length ξ. An alternative picture was suggested in [4] and further developed in [8]. It concentrates on effects that persist even at zero temperature and are due to a strong interaction between bare electronic excitations and perturbations (the amplitude and phase phonons) of the CDW ground state. Here, the pseudogap in instantaneous electronic spectra is related to the transformation of electrons into solitons.

Experimentally, pseudogaps in incommensurate CDWs were first addressed by optic [9–11] and more recently by the PES and ARPES (momentum-resolved PES) methods [12]. The earlier experiments were theoretically interpreted in [13] by compilation of the approaches in [3, 4, 7]. Detailed theories of the subgap absorption in optics have been developed for systems with low symmetries (nondegenerate, like semiconductors with gapful phonons, or discretely degenerate like the dimerized Peierls state). They first addressed the general type of polaronic semiconductors [14] with emphasis on long-range Coulomb effects, and then the $1D$ Peierls system, emphasizing solitonic processes (see [15] and references therein). The authors recently [1] extended the theory of pseudogaps to single electronic spectra in application to PES, and particularly intriguing, to ARPES probes. But properties of incommensurate CDWs are further complicated by the appearance of a gapless collective mode resulting in drastic changes. The case of acoustic polarons in a $1D$ semiconductor belongs to the same class, although this is not usually noticed.

A specific property of $1D$ systems with continuous degeneracy (with respect to the phase for incommensurate CDWs and to displacements for usual crystals) is that even a single electronic process can create topologically nontrivial excitations, solitons. For incommensurate CDWs, a single electron or hole with the energy near the gap edges $\pm\Delta_0$ spontaneously evolves to a nearly amplitude soliton while the original particle is trapped at the local level near the gap center. The energy near $0.3\Delta_0$ is released, at first sight, within the time $\omega_{ph}^{-1} \sim 10^{-12}$ s. We see in what follows that there actually also exists a long-scale adaptation process that determines shapes of transition probabilities. Similarly, the usual acoustic polaron in $1D$ semiconductors is characterized by the electronic density $\rho \sim \partial\varphi/\partial x$ self-localized within the potential well, and hence, there is a finite increment $\varphi(+\infty) - \varphi(-\infty) \sim \int \rho dx$ of the lattice displacements φ over the length x, which is the signature of topologically nontrivial solitons. These systems with continuous degeneracy form a special class that shows particular properties and must be studied differently than in [1]. They are addressed in this paper.

2. FUNCTIONAL INTEGRALS AND INSTANTONS FOR PES

As a function of the frequency Ω and momentum P, the absorption rate $I(\Omega, P)$ for ARPES can be expressed in terms of the spectral density of the one-electron retarded Green's function $G(t, t'; x, x')$ as

$$I(P,\Omega) \propto \mathrm{Im} \int dX e^{-iPX} \int_0^\infty dT e^{i\Omega T} G(X,T,0,0). \quad (1)$$

We here address the simple PES, not resolved in momenta, which measures the integrated absorption intensity

$$I(\Omega) = \frac{1}{2\pi} \int I(P,\Omega) dP.$$

(From now on, we omit all constant factors and set the Planck constant $\hbar = 1$; Ω is then measured with respect to a convenient level, the band edge for semiconductors or the middle of the gap for CDWs.)

We use the adiabatic approximation, which is valid when changes of electronic energies are much larger than the relevant phonon frequencies. Electrons move in a slowly varying phonon potential, e.g., $\mathrm{Re}[\Delta(x,t)\exp(2ik_F x)]$ for an incommensurate CDW, and at any instant t their energies $E(t)$ and wave functions $\psi(x,t)$ are therefore defined as eigenstates for the instantaneous lattice configuration and depend on time only parametrically. In what follows, we work in the Euclidean space $it \to t$, which is adequate for studies of classically forbidden processes [14, 16, 17]. The integrated absorption intensity is then given by a functional integral over lattice configurations,

$$I(\Omega) \propto \int_0^\infty dT \int D[\Delta(x,t)] \psi_0(0,T) \psi_0^+(0,0) e^{-S}, \quad (2)$$

where ψ_0 is the wave function of the particle (which is actually a hole for PES) added and extracted at moments 0 and T. Only the lowest singly filled localized state is relevant for calculations of subgap processes. The energy E_0 of this state is split inside the gap. The action

$$S = S[\Delta(x,t),T] = \left(\int_{-\infty}^{0} + \int_{T}^{\infty}\right) dt\, L_0 + \\ + \int_{0}^{T} dt\,(L_1 - \Omega), \quad L_1 - L_0 = E_0 \quad (3)$$

is expressed through the Lagrangians $L_j[\Delta]$, where the subscripts $j = 0, 1$ correspond to ground states for $2M$ (the bare number) and $2M \pm 1$ electrons in the potential $\Delta(x,t)$. The main contribution comes from saddle points of S, the instantons, which are extremums with respect to both the function $\Delta(x,t)$ and the time T. There are also special cases [1], particularly important for ARPES, where the extremum must be taken for the entire integrand in (2), with the wave functions in the prefactor taken into account. Otherwise, the stationary point is determined by $dS/dT = 0$, that is, $E_0(0) = E_0(T) = \Omega$, which determines $T(\Omega)$.

In what follows, we concentrate on most principal features, leaving aside calculations of prefactors and the problem of the momentum dependence necessary for ARPES. For a simpler case of nondegenerate systems, they have been studied in [1].

3. CREATION OF AMPLITUDE SOLITONS IN INCOMMENSURATE CDWs

We first consider the subgap electronic spectra for the incommensurate CDW described by the Peierls–Fröhlich model. The incommensurate CDW order parameter is the complex field $\Delta = |\Delta(x,t)| \exp[i\varphi(x,t)]$ acting on electrons by mixing states near the Fermi momenta points $\pm k_F$. The Lagrangians L_j consist of the bare kinetic and potential lattice energies and of the sum over the filled electron levels, in the jth state,

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

where v_F is the Fermi velocity in the metallic state and ω_0 is the amplitude mode frequency ($\omega_0 \ll \Delta_0$ is the condition for the adiabatic approximation).

The important fact is that the stationary state of the system with an odd number of particles, the minimum of V_1, is an amplitude soliton, with the midgap state $E_0 = 0$ occupied by a singe electron. Evolution of the free electron with the initial energy $E_0 = \Delta_0$ to the amplitude soliton with $W_s = 2\Delta_0/\pi < \Delta_0$

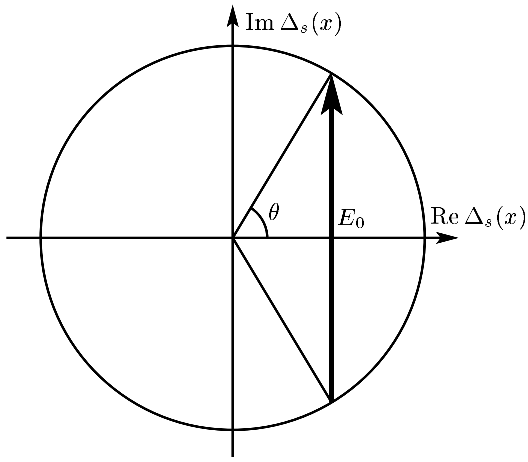

Fig. 1. Trajectory of the chordus soliton with phase tails in the complex plane Δ

can be described by the known exact solution for intermediate configurations characterized by the single intragap $E_0 = \Delta_0 \cos\theta$ with $0 \le \theta \le \pi$, whence $-\Delta_0 \le E_0 \le \Delta_0$. It was found [8] (see also reviews [18, 19]) to be the chordus soliton with 2θ as the total chiral angle, $\Delta(+\infty)/\Delta(-\infty) = \exp(2i\theta)$, see Fig. 1 and the Appendix for details. The filling numbers $\nu = 0, 1$ of the intragap state correspond to labels $j = 0, 1$. The term $V_0(\theta)$ monotonically increases from $V_0(0) = 0$ for the $2M$ ground state to $V_0(\pi) = 2\Delta_0$ for the $2M + 2$ ground state with two free holes. The term $V_1(\theta) = V_1(\pi - \theta)$ is symmetric and describes both a particle on the $2M$ ground state and a hole on the $2M + 2$ ground state. Obviously, $V_1(0) = V_1(\pi) = \Delta_0$, while the minimum is reached at $\theta = \pi/2$, that is for a purely amplitude solution: $\min V(\theta) = V_1(\pi/2) = W_s < \Delta_0$, where $W_s = 2\Delta_0/\pi$ is the amplitude solution energy, see Fig. 2. Therefore, to create a nearly amplitude soliton with $\theta = 90°$, 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 $\theta \approx 50°$.

We note that the amplitude soliton, being an uncharged spin carrier with the topological charge one, is a quasiclassical realization of a spinon in systems with nonretarded attraction of electrons (that is, with high, rather than low, phonon frequencies). Therefore, our analysis is also qualitatively applied to arbitrary nonadiabatic electronic systems provided they are found in the spin-gap regime. (See also the next section.)

It is tempting to use the static solution, with some free parameter, as an ansatz for the time-dependent process; this proved to be successful in gapful cases

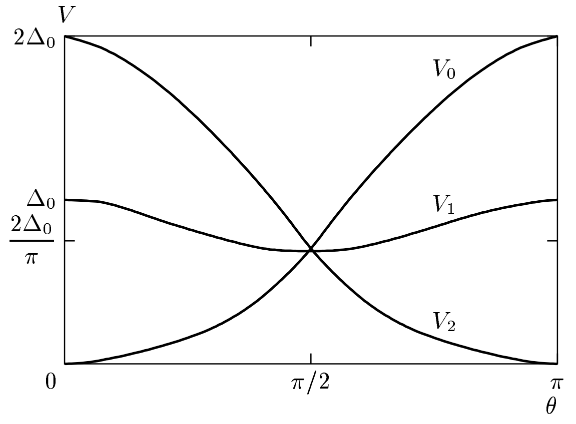

Fig. 2. Selftrapping terms V_ν for chordus solitons as functions of the chiral angle 2θ for various fillings ν

[1, 15]. But here, putting $\theta \to \theta(t)$, we would arrive at $\partial_t \Delta \neq 0$ for all x, and the action would therefore be infinite, S is proportional to the system length. The vanishing probability simply reflects the fact that a globally finite perturbation, characteristic of topologically nontrivial solitons, cannot spread over the whole length in a finite time. More generally, as a topologically nontrivial object, the amplitude soliton cannot be created in a pure form: adaptational deformations must appear to compensate the topological charge. These deformations develop over long space–time scales and can be described in terms of the gapless mode, the phase φ, alone. Allowing the time evolution of the chiral angle $\theta \to \theta(t)$ within the core, we must therefore also unhinder the field $\varphi \to \varphi(x,t)$ for all x and t. The resulting trajectory is shown in Fig. 1 for an instant of time. Starting from $x \to -\infty$ and returning to $x \to \infty$, the configuration closely follows the circle $|\Delta| = \Delta_0$ changing almost entirely by phase. Approaching the soliton core, the phase approximately matches the angles $\pm\theta$ that delimit the chordus part of the trajectory. The entire trajectory is closed, which leads to a finite action.

Except for a short time scale $T < \xi_0/u$ (see Sec. 4.2) characterized by small θ and large lengths $\xi = \xi_0/\sin\theta$, the configuration $\Delta(x,t)$ can be divided into the inner part, the core at $|x| \sim \xi$, and the outer part $|x| \gg \xi$, where only perturbations of the phase $\varphi(x,t)$ are important. The inner part can be described by the chordus soliton $\Delta_{\text{ChS}}(x,t)$. The chordus angle $2\theta(t)$ evolves in time from $\theta(\pm\infty) = 0$ to θ_m in the middle of the T interval. As $T \to \infty$, that is, near the stationary state of the amplitude soliton, $\theta_m \to \pi/2$. This value is actually preserved during most of the T interval, and the changes between $\theta = 0$ and $\theta = \pi/2$ are therefore concentrated within finite ranges $\tau_0 \sim \xi_0/u \ll T$ near the termination points. At large scales, we can see only a jump $\varphi(x,t) \approx \theta(t)\,\mathrm{sign}\,x$ with $\theta(t) \approx \theta_m \Theta(t)\Theta(T-t)$, where Θ is the standard step function. Because the configuration stays close to the amplitude soliton during the time T, the main core contribution to the action is

$$S_{core} = (W_s - \Omega)T + \delta S_{core}, \tag{4}$$

where the first correction $\delta S^0_{core} = \text{const}$ comes form regions around the instants 0 and T independently. The significant T-dependent contribution $\delta S(T)$ comes from interference of regions 0 and T. Their interaction via gapful excitations like the amplitude mode decays exponentially as $\delta S_{gap} \propto \exp(-\omega_0 T)$. There are no other contributions for low-symmetry systems, but for an incommensurate CDW, there are sound modes providing the main effect to be addressed below.

Matching the inner and outer regions is not well defined unless we consider the full microscopic time-dependent model, which is impossible. But fortunately, the long-range effects can be treated easily if we generalize the scheme suggested earlier for static problems of solitons in the presence of interchain interactions [8, 20]. The outer region is described by the action for the sound-like phase mode,

$$S_{snd}[\varphi(x,t),\theta(t)] = \\ = \frac{v_F}{4\pi}\iint dx\,dt\left[\left(\frac{\partial_t\varphi}{u}\right)^2 + (\partial_x\varphi)^2\right], \tag{5}$$
$$\varphi(t, x_s \pm 0) = \mp\theta(t),$$

where u is the phase velocity. The conditions on φ at $x_s \pm 0$ are due to the source provided by the chordus soliton that is formed around x_s and enforces the discontinuity 2θ. Integrating $\exp[-S_{snd}(\varphi,\theta)]$ over $\varphi(x,t)$ with this condition, we arrive at the action for $\theta(t)$,

$$S_{snd}[\theta] \approx \frac{v_F}{2\pi^2 u}\iint dt_{1,2}\dot\theta(t_1)\ln|(t_1-t_2)|\dot\theta(t_2) = \\ = \frac{v_F}{2\pi^2 u}\iint dt_{1,2}\left(\frac{\theta(t_1)-\theta(t_2)}{t_1-t_2}\right)^2. \tag{6}$$

The last form of this action is typical of the quantum dissipation problem [21], where $S \sim \sum|\omega||\theta_\omega|^2$. In our case, this dissipation arises from the emission of phase phonons forming a long-range tail in the course of the chordus soliton development. Together with V_j, this action can be used to prove the above statements on the time evolution of the chordus soliton core.

We now recall that $\dot\theta = \partial_t\theta$ is peaked within narrow regions of the order of ξ_0/u around the time instants $t = 0$ and $T = 0$ and is close to zero elsewhere. Then

$$S_{snd} \approx \frac{v_F}{4u} \ln \frac{uT}{\xi_0}. \quad (7)$$

There is an even more phenomenological standpoint (see [22] for more details and examples of combined topological defects). The amplitude soliton creates the π-discontinuity along its world line $(0 < t < T, 0)$. To be topologically allowed, that is, to have a finite action, the line must terminate with half integer vortices located at $(0,0)$ and $(0,T)$, whose circulation must provide the compensating jump $\delta\varphi = \pi$ along the interval ($\Delta \to -\Delta$ combined with $\varphi \to \varphi + \pi$ leaves the order parameter $\Delta\exp(i\varphi)$ invariant). The standard energy of vortices for (5) then leads to action (7). Contrary to the usual 2π-vortices, the line connecting the half-integer ones is a physical singularity whose tension gives (4).

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

$$I(\Omega) \propto \left(\frac{\Omega - W_s}{W_s}\right)^\beta, \quad \beta = \frac{v_F}{4u}, \quad (8)$$

which is much more pronounced than the exponential law for gapful cases (see (15) below).

Our derivation suggests a literal long-range order at large (x,t) distances and neglects all fluctuations of the phase except perturbations enforced by the instanton. But the mean fluctuations of the phase diverge and the order parameter decays in accordance with a power law. These long-range fluctuations are not related to the instanton and can be taken into account *a posteriori*. This can be easily done by noticing that the eigenfunctions in the prefactor in (2) transform as $\Psi_0 \to \Psi_0 \exp[i\varphi(x,t)/2]$, and being averaged, contribute the action term

$$\delta S_\varphi = \frac{1}{8}\langle[\varphi(0,0) - \varphi(0,T)]^2\rangle \approx \frac{u}{4v_F} \ln \frac{uT}{\xi_0}.$$

Therefore, the effect of phase fluctuations, as well as the major role of the formfactor, is simply a correction to the value of the index in (8), $\beta \to \beta^* = v_F/4u + u/4v_F$. Within our adiabatic approximation $u/v_F \ll 1$, the correction is small but it builds a bridge to quantum nonadiabatic models where exactly β^* appears as the index of the single-particle Green's function with $\gamma_\rho = u/v_F$ identified as the charge channel exponent. The link is completed by noting that the amplitude soliton is a realization of the spinon and that the phase discontinuity in (5) is equivalent, together with fluctuations, to applying the operator

$$\exp\left\{\frac{i}{2}\varphi(x,t) + i\frac{\pi}{2}\frac{\delta}{\delta\varphi} \operatorname{sign} x\,\Theta(t)\Theta(T-t)\right\},$$

which is our limit for bosonization.

4. ACOUSTIC POLARON AND THE FREE EDGE

4.1. 1D semiconductors with acoustic and optical polarons

Behavior near the free edge $\Omega \approx \Delta_0$ is dominated by small fluctuations η in the gap amplitude, $|\Delta| = \Delta_0 + \eta$, and at the Fermi level, $\delta E_F = \varphi' v_F/2$, via the phase gradient $\varphi' = \partial_x\varphi$. We consider it in the framework of the general problem of a combined (gapful and acoustic) polaron. The more simple, compared to the CDW, single-particle formulation bears similar qualitative features but allows a more detailed analysis. We consider electron (hole) states in a 1D dielectric near the edge of a conducting (valence) band. We account for the gapful mode η with the coupling g_0 and the sound mode (for which we keep the «phase» notation φ) with the velocity u and the coupling g_s. In generic semiconductors, the sound mode is always present as the usual acoustic phonon, while the gapful mode can be present as an additional degree of freedom. In all CDWs, the gapful mode is always present as the amplitude fluctuation $|\Delta| = \Delta_0 + \eta$, while the sound mode appears in incommensurate CDWs as the phase $\Delta = |\Delta|\exp(i\varphi)$.

Within the adiabatic approximation for the electron wave function Ψ, the action S (at imaginary time) is given by

$$\begin{aligned} S = \int dx \int_0^T dt \left\{ \left(\frac{1}{2m}|\partial_x\Psi|^2 - \Omega|\Psi|^2\right) + \right. \\ \left. + \left(g_s\partial_x\varphi + g_0\eta\right)\Psi^\dagger\Psi \right\} + \\ + \int dx \int_{-\infty}^{\infty} dt \left\{\frac{K_s}{2}\left[\left(\frac{\partial_t\varphi}{u}\right)^2 + (\partial_x\varphi)^2\right] + \right. \\ \left. + \frac{K_0}{2}\left[\left(\frac{\partial_t\eta}{\omega_0}\right)^2 + \eta^2\right]\right\}. \end{aligned} \quad (9)$$

For the incommensurate CDW case, we therefore have $m = \Delta_0/v_F^2$, $g_0 = 1$, $g_s = v_F/2$, $K_s = v_F/2\pi$, $K_0 = 4v_F/\pi$, $2^{3/2}u/v_F = \omega_0/\Delta_0$, and Ω is counted with respect to the edge Δ_0 rather than to the middle of the gap as in the previous section.

It is well known [5] that the stationary state, i.e., the time-independent extremum of (9), corresponds to the selftrapped complex, the polaron. Here, it is composed equally by η and φ', which contribute additively to the static coupling (while the dynamics is completely different):

$$\lambda = \lambda_s + \lambda_0 = \frac{g_s^2}{K_s} + \frac{g_0^2}{K_0}.$$

The polaronic length scale l for $\eta \sim \varphi' \sim |\Psi|^2 \equiv \rho_p(x)$ is $l = 2\lambda/m$ 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, Born–Oppenheimer, approximation. For the CDW case, $\lambda_s = v_F\pi/2$ and $\lambda_0 = v_F\pi/4$, and therefore, $\lambda \sim v_F$ and we 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 can be used only qualitatively. The full-scale approach for nearly stationary states was considered in Sec. 3, but the upper pseudogap region near the free edge Δ_0 is described by model (9) even quantitatively and most efficiently.

We can integrate over the fields φ and η at all (x,t) to obtain the action in terms of ψ alone, which is now defined only on the interval $(0,T)$ for t,

$$\begin{aligned} S\{\Psi;T\} = \int dxdt \left(\frac{1}{2m}|\partial_x\Psi|^2 - \Omega|\Psi|^2\right) - \\ - \frac{1}{2}\iint dt_{1,2}\iint dx_{1,2} \times \\ \times \{U_0(x_1-x_2,t_1-t_2)\rho(x_1,t_1)\rho(x_2,t_2) + \\ + U_s(x_1-x_2,t_1-t_2)\partial_x\rho(x_1,t_1)\partial_x\rho(x_2,t_2)\}. \end{aligned} \quad (10)$$

Here, the retarded self-attraction potentials are

$$\begin{aligned} U_s &= \frac{\lambda_s u}{2\pi}\ln\sqrt{x^2+t^2u^2}, \\ U_0 &= \frac{1}{2}\lambda_0\omega_0\exp[-\omega_0|t|]\delta(x). \end{aligned} \quad (11)$$

An equivalent form, suitable at large T, is obtained via integrating by parts,

$$\begin{aligned} S\{\Psi;T\} = \int dx\int_0^T dt\left[\frac{1}{2m}|\partial_x\Psi|^2 - \Omega\rho - \frac{\lambda}{2}\rho^2\right] + \\ + \frac{1}{2}\iint dt_{1,2}\iint dx_{1,2}\partial_t\rho(x_1,t_1)\partial_t\rho(x_2,t_1) \times \\ \times U(x_1-x_2,t_1-t_2), \end{aligned} \quad (12)$$

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 long-time processes when the lattice configuration is almost statically self-consistent. The first term in (12) is nothing but the action S_{st} of the static polaron whose extremum at a given T is

$$S_{st} \approx -T\delta\Omega, \quad \delta\Omega = \Omega - W_p.$$

The second term in (12), S_{tr}, collects contributions only from short transient processes near the impact moments $t = 0, T$, which are seen by the long-length part as $\partial_t\rho(x,t) \approx \rho_p(x)[\delta(t) - \delta(t-T)]$, where ρ_p is the density for the static polaron solution. We obtain

$$\begin{aligned} S_{tr} &\approx \iint dx_{1,2}\rho_p(x_1)\rho_p(x_2)U(x_1-x_2,T) = \\ &= \frac{\lambda_s}{2\pi u}\ln\frac{uT}{l} + C_0\frac{\lambda_0/l}{\omega_0}\exp(-\omega_0 T) + \text{const} \end{aligned}$$

with $C_0 \sim 1$. We see the dominant contribution of the sound mode that grows logarithmically in T, while the part of the gapful mode decays exponentially. If the sound mode is present, the extremum over T is

$$T \approx \frac{\lambda_s}{2\pi u}\frac{1}{\delta\Omega}, \quad S \approx \frac{\lambda_s}{2\pi u}\ln\frac{C_s|W_p|}{\delta\Omega}, \quad C_s \approx 0.9. \quad (13)$$

We find that near the absolute edge $\Omega \approx W_p$, the absorption is given by a power law with the index α that must be large within our adiabatic assumption, $\alpha \gg 1$,

$$I \sim \left(\frac{\delta\Omega}{|W_p|}\right)^\alpha, \quad \alpha = \frac{\lambda_s}{2\pi u}. \quad (14)$$

For incommensurate CDW parameters, we obtain $\alpha = v_F/4u$, in full accordance with the exact treatment (8).

Only in the absence of sound modes, $\lambda_s = 0$, the gapful contribution can determine the absolute edge. Minimization of $S = S_{core} + \delta S_{gap}$ over T then leads qualitatively to the result in [1],

$$\begin{aligned} T &\sim \omega_0^{-1}\ln\left|\frac{W_p}{W_p-\Omega}\right|, \\ I &\propto \exp\left(-\text{const}\cdot\frac{|W_p|}{\omega_0} + \frac{\Omega-W_p}{\omega_0}\ln\left|\frac{W_p}{\Omega-W_p}\right|\right) \end{aligned} \quad (15)$$

for $\Omega \approx W_p$.

4.2. Free-electron edge vicinity

We now consider the opposite regime near the free edge $\Omega \approx 0$ ($\Omega \to \Omega - \Delta_0$ for the incommensurate CDW). Here, entering the pseudogap at $\Omega < 0$, the absorption is determined by fast processes of quantum fluctuations: their characteristic time $T = T(\Omega)$ is short compared to the relevant phonon frequency, $T \ll \omega_0, u/L$, where $L = L(\Omega)$ is the characteristic localization length for the fluctuational electron level at $E_0 = \Omega$. Because T is small, we can neglect all variations in time within $(0, T)$. We then estimate action (10), term by term, as

$$S \approx \frac{C_1 T}{mL^2} - \Omega T - C_2 \lambda_s u \left(\frac{T}{L}\right)^2 - C_3 \lambda_0 \omega_0 \frac{T^2}{L}, \quad (16)$$

where $C_i \sim 1$. The condition for its extremum with respect to both L and T yields

$$S \sim \frac{|\Omega|^{3/2}/m^{1/2}}{\max\left\{|m\Omega|^{1/2} u \lambda_s; \omega_0 \lambda_0\right\}},$$

which provides a reasonable interpolation for the absorption in the closest and the more distant vicinities of the free-electron edge. For the purely acoustic case $\lambda_0 = 0$, a variational estimation of the numerical coefficient as $C_1 \approx 1/6, C_2 \approx 0.06$ gives

$$I \propto \exp(-\text{const} \cdot |\Omega|/mu\lambda_s), \quad \text{const} \approx 2.8. \quad (17)$$

The validity condition $uT/L \sim \sqrt{-\Omega/W_p} \ll 1$ is satisfied by definition of the edge region. This condition is compatible with the low boundary for the frequency, $S \gg 1$, and hence, $-\Omega/W_p \gg u/\lambda_s$, which is small as our basic adiabatic parameter.

For gapful phonons alone, $\lambda_s = 0$ and we arrive at the known result

$$I \propto \exp[-\text{const} \cdot |\Omega|^{3/2}/\omega_0], \quad \Omega < 0$$

(see [1] and references therein). But it was not quite predictable that among the laws $S \propto |\Omega|^{3/2}$ and $S \propto |\Omega|$, it is the smallest contribution to S that wins, proportional to $|\Omega|^{3/2}$ at lowest $|\Omega|$ and to $|\Omega|$ for larger $|\Omega|$. For the incommensurate CDW, in particular, we have $\lambda_0/\lambda_s \sim 1$ and $u/\omega_0 \sim \xi_0$, and there is no space for the intermediate asymptotic regime $\ln I \propto \Omega$ at $|\Omega| \ll \Delta_0$: beyond the region with $S \propto |\Omega|^{3/2}$, the amplitude fluctuations dominate, the phase-only description is invalid, and the particular nature of amplitude solitons must be taken into account. This regime was considered in Sec. 3.

The difference between the laws $\ln I \propto -|\Omega|/u$ and $\ln I \propto -|\Omega|^{3/2}/\omega_0$ can be interpreted easily. Indeed, for gapful phonons, we expect the frequency scale to be $\omega_0 \to \omega_k = uk \sim u/L \sim u|\Omega|^{1/2}$, where $k \sim 1/L$ is a characteristic wave number and L is the localization length of the fluctuation providing the bound state at $-\Omega$. Then $|\Omega|^{3/2}/\omega_0 \to |\Omega|^{3/2}/\omega_k \sim |\Omega|/u$.

While law (17) appears to be the simplest one, it is actually quite uncommon and its derivation is problematic in all systems, cf. [14]. In our case, we note that only at $\lambda_0 \neq 0$, action (16) has the usual saddle point, a minimum over L and a maximum over T. But for the purely acoustic case $\lambda_0 = 0$, the minimum over L appears only along the extremal line over T. Contrarily, at a given T, the action collapses to either $L \to 0$ or $L \to \infty$ depending on the value of T with respect to the threshold $T^* \sim (mu\lambda_s)^{-1}$, which is just the inverse width in (17). The paradox can be resolved by inspecting the generic real time formulation (2). But the necessary insight is obtained more easily by another treatment presented in the next section.

4.3. Quantum fluctuations as an instantaneous disorder with long-range space correlations

It has already been noticed that in a $1D$ system, the optical absorption near the band edge can be viewed as for a quenched disorder emulated by instantaneous quantum fluctuations. This asymptotically exact reduction to the time-independent model can be done as follows. After neglecting the retardation at $T \ll \omega_0, u/L$, the self-interaction term in (10) can be decoupled by the Hubbard–Stratonovich transformation via a time-independent field ζ with the correlator $D(x) = U_0(x,0) + \partial_x^2 U_s(x,0)$,

$$S\{\Psi, \zeta; T\} = T \int dx \left(\frac{1}{2m} |\partial_x \Psi|^2 + \zeta(x)\rho(x)\right) + \\ + \frac{1}{2} \iint dx_{1,2} \zeta(x_1) D^{-1}(x_1 - x_2) \zeta(x_2). \quad (18)$$

After integration over Ψ and rotation to the real time, it finally becomes the density of states

$$\int D[\zeta(x)] \delta(E[\zeta(x)] - \Omega) \times \\ \times \exp\left[-\frac{1}{2} \iint dx_1 dx_2 \zeta(x_1) D^{-1}(x_1 - x_2) \zeta(x_2)\right],$$

where $E[\zeta(x)]$ is the eigenfunction in the random field ζ,

$$-\frac{\partial_x^2}{2m}\Psi + \zeta\Psi = E\Psi.$$

For the dispersionless phonon alone, e.g., the amplitude mode in the CDW, $D(x) = U_0(x,0) \sim \delta(x)$, and the known exact results for the uncorrelated disorder [23] provide us with the asymptotic pseudogap formula

$$I(\Omega) \propto \exp\left[-\frac{8}{3^{3/2}} \frac{|W_p|}{\omega_0} \left|\frac{\Omega}{W_p}\right|^{3/2}\right]. \quad (19)$$

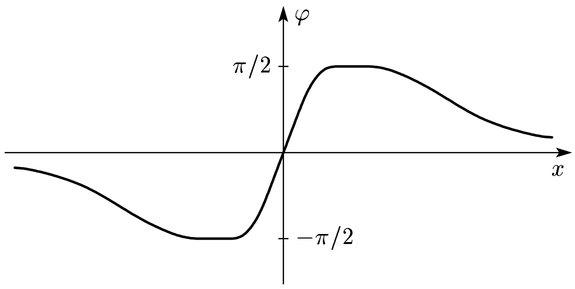

Fig. 3. The acoustic polaron field $\varphi(x,t)$ as a function of x at some moment t

For the CDW parameters, it becomes

$$I(\Omega) \propto \exp\left[-\frac{16}{3\pi}\left(2\frac{\Delta_0-\Omega}{(\Delta_0\omega_0^2)^{1/3}}\right)^{3/2}\right]. \qquad (20)$$

Below, we concentrate only on a more problematic case of the sound mode. The correlator $D(x)$ of the «disordered potential» ζ is just the mean square of quantum fluctuations of the phonon potential $\zeta = v_F/2\varphi'(x,t)$ at coinciding times: in the Fourier representation, we have

$$D_k = \int \frac{d\omega}{2\pi}\frac{\lambda_s k^2}{(\omega/u)^2+k^2} = \frac{1}{2}\lambda_s u|k|\,.$$

The probability distribution for the Fourier components ζ_k is

$$P[\zeta_k] \propto \exp\left(-\int\frac{dk}{2\pi}\frac{|\zeta_k|^2}{\lambda_s u|k|}\right), \qquad (21)$$

which implies that the component with $k=0$ is excluded, $P(\zeta_0)=0$. The constraint

$$\zeta_0 = \int\limits_{-\infty}^{\infty}\zeta(x)dx = 0 \qquad (22)$$

agrees with the properties of the potential proportional to φ' in the time-dependent picture of the previous section, which satisfies condition (22) at any finite t, see Fig. 3. Contrary to the usual expectations of the method of optimal fluctuations, the potential well creating the level E must here be accompanied by compensating barriers. Condition (22) is linked to the paradox in the pervious section, i.e., the absence of a finite minimum over the length scale at a given T. Indeed, we can no longer rely on the existence of a bound state at an arbitrarily shallow potential, $E_0 \sim -m\left(\int dx\zeta(x)\right)^2$, which is zero under condition (22).

While the divergency at small k (large x) is physical, the one at large k in (21) must be regularized to apply in the real space. We proceed by introducing an auxiliary field $\mu(x)$ such that $\zeta = d\mu/dx = \mu'$. We finally arrive at the model of the «nonlocal acoustic disorder»,

$$I(\Omega) \propto \int D[\mu(x)]\delta(E[\partial_x\mu(x)]-\Omega)\times$$
$$\times\exp\left[-\frac{\lambda_s}{2u}\iint dx_1dx_2\frac{(\mu(x_1)-\mu(x_2))^2}{|x_1-x_2|^2}\right]. \qquad (23)$$

Here, the integral in the exponent is already regular at small x. The divergence at large x maintains constraint (22), otherwise

$$\mu(+\infty)-\mu(-\infty) = \int\limits_{-\infty}^{\infty}\zeta(x)dx \neq 0$$

and the integral in (23) would diverge logarithmically, leading to zero probability.

Unfortunately, we are unaware of exact studies for disordered systems with such long-range correlations. Usual scaling estimations [24] for characteristic μ and l give $|\Omega| \sim 1/ml^2 \sim |\mu|/l$, then $|\mu| \sim |\Omega/m|^{1/2}$, and therefore, $\ln I \sim -\mu^2\lambda_s/u \sim -|\Omega|\lambda_s/u$, in accordance with direct estimations and result (17) for the general time-dependent model.

5. DISCUSSION AND CONCLUSIONS

We summarize the obtained results as follows.

The pseudogap starts below the free edge by (stretched) exponential dependences

$$I \propto \exp\left[-\text{const}\cdot(-|\Omega|)^\gamma\right] \qquad (24)$$

with different powers $\gamma = 3/2$ for gapful phonons and $\gamma = 1$ for sound photons. If both modes are present, then the smallest one, with $\gamma = 3/2$, dominates at small Ω. This regime corresponds to free electronic states smeared by instantaneous uncorrelated quantum fluctuations of the lattice.

Deeply within the pseudogap, approaching the absolute threshold W_s or W_p, the exponential law changes for the power law $I(\Omega) \propto (\Omega - W_s)^\beta$ with a large exponent β. This contribution dominates over the smooth one from gapful modes $I \propto \exp(\text{const}\cdot\delta\Omega\ln\delta\Omega)$. The power-law regime corresponds to creation of nearly amplitude solitons surmounted be compensating phase tails. Its description provides a semiclassical interpretation for processes in fully quantum systems of correlated electrons in the spin-gap regime, with the amplitude soliton being a version of the spinon.

These results are different from anything used earlier in either theoretical discussions or interpretation of experimental data [13]. They can vaguely explain unusually wide pseudogaps observed in experiments even at low temperatures for well-formed incommensurate CDWs.

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 incommensurate CDWs, the results are applied to a vicinity of the free edge. But the edge at $2E_s$ disappears in favor of the optically active gapless phase mode.

We empliasize in this respect that there cannot be a common pseudogap for processes characterized by different time scales. We must distinguish [8] between short-living states observed in optical, PES (and maybe tunneling) experiments and long-living states (amplitude solitons and phase solitons) contributing to the spin susceptibility, NMR relaxation, heat capacitance, conductivity, etc. States forming the optical pseudogap are created instantaneously; particularly near the free edge, they are tested over times that are shorter than the inverse phonon frequencies $\tau_{opt} \sim \hbar/E_g < \omega_{ph}^{-1}$ and many orders of magnitude beyond the lifetimes required for current carriers, and even much longer times for thermodynamic contributions. It then follows that the analysis of different groups of experimental data [13] within the same picture must be reconsidered. The lack of discriminating different time scales also concerns typical discussions of pseudogaps in high-T_c superconductors.

We conclude that the subgap absorption in systems with gapless phonons is dominated by formation of long space–time tails of relaxation. It applies to both acoustic polarons in $1D$ semiconductors and solitons in CDWs. Near the free edge, a simple exponential, Urbach-type law appears competing with stretched exponential laws of tails from optimal fluctuations. A deeper part of the pseudogap is dominated by a power-law singularity near the absolute edge.

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APPENDIX

Electronic energies in a complex field Δ are determined by the Dirac Hamiltonian

$$\begin{vmatrix} -iv_F\partial_x & \Delta \\ \Delta^* & iv_F\partial_x \end{vmatrix}, \quad \Delta = |\Delta| e^{i\varphi}.$$

In the ground state, $|\Delta(x,t)| = \Delta_0$, we have $\varphi = \text{const}$, and the electronic spectrum is $E^2 = v_F^2 k^2 + \Delta_0^2$, where v_F is the Fermi velocity. But these free states are not proper excitations. The evolution of added electrons or holes with the initial energy $E_0 \geq \Delta_0$ to the amplitude soliton with $W_s = 2\Delta_0/\pi < \Delta_0$ can be described by an exact solution for intermediate configurations characterized by the singly occupied arbitrary positioned intragap state $E_0 = \Delta_0 \cos\theta$ with $0 \leq \theta \leq \pi$, whence $-\Delta_0 < E_0 < \Delta_0$. It was found [8] to be the chordus soliton with 2θ being the total chiral angle, $\Delta(\pm\infty) = \exp(\pm i\theta)$, see Fig. 1. Namely,

$$\Delta_{ChS}(x,\theta) = \Delta_0[\cos\theta + i\sin\theta\,\mathrm{th}(k_0 x)]\exp(i\varphi_0), \quad k_0 = \Delta_0 \sin\theta \tag{25}$$

with an arbitrary $\varphi_0 = \text{const}$. The potentials V_ν are known [8] to be given by (see Fig. 2)

$$V_\nu(\theta) = \Delta_0 \left[\left(\nu - \frac{2}{\pi}\theta \right) \cos\theta + \frac{2}{\pi}\sin\theta \right],$$

where ν is the filling number of the intragap state, that is, $\nu = 0, 1$ for $j = 0, 1$ while $\nu = 2$ is equivalent to $j = 0$ for the ground state extended by the two particles, $N = 2M + 2$. The term $V_0(\theta)$ monotonically increases from $V_0(0) = 0$ for the $2M$ ground state to $V_0(\pi) = 2\Delta_0$ for the $2M + 2$ ground state with two free holes. Obviously, there is an opposite dependence for $V_2(\theta) = V_0(\pi - \theta)$. Therefore, the total phases slip $2\theta = 0 \to 2\theta = 2\pi$ realizes the spectral flow across the gap, also accompanied by the flow of particles for $\nu = 2$ that makes it favorable. The term $V_1(\theta) = V_1(\pi - \theta)$ is symmetric and describes both the particle on the $2M$ ground state and the hole on the $2M + 2$ ground state. Apparently, $V_1(0) = V_1(\pi) = \Delta_0$ (the degenerate ground states are the $2M$ one with an additional free electron for $\theta = 0$ and the $2M + 2$ one with an additional free hole for $\theta = \pi$), while the minimum is $V_1(\pi/2) = W_s < \Delta_0$, where $W_s = 2\Delta_0/\pi$ is the amplitude soliton energy. Therefore, the stationary state of the system with an odd number of particles, the minimum of V_1, is the amplitude soliton with the midgap state $E_0 = 0$ occupied by a singe electron.

We note that being an uncharged spin carrier with the topological charge equal to unity, the amplitude soliton is a semiclassical realization of a spinon in systems with nonretarded attraction of electrons (that is, with high, rather than low, phonon frequencies).

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