Subgap tunneling through channels of polarons and bipolarons in chain conductors

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We suggest a theory of internal coherent tunneling in the pseudogap region where the applied voltage is below the free electron gap. We consider quasi-one-dimensional (1D) systems where the gap is originated by a lattice dimerization (Peierls or SSH effect) as in polyacethylene, as well as low symmetry 1D semiconductors. Results may be applied to several types of conjugated polymers, to semiconducting nanotubes, and to quantum wires of semiconductors. The approach may be generalized to tunneling in strongly correlated systems showing the pseudogap effect, as in the family of high-T_c materials in the undoped limit. We demonstrate the evolution of tunneling current-voltage characteristics from smearing the free electron gap down to threshold for tunneling of polarons and further down to the region of bielectronic tunneling via bipolarons or kink pairs. The interchain tunneling is described in a parallel comparison with the on chain optical absorption, also within the subgap region.

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I. INTRODUCTION

The interchain, interplane transport of electrons in low-dimensional [quasi-one-dimensional (1D), quasi-2D] materials attracts much attention[1] in view of striking differences between longitudinal and transverse transport mechanisms revealing a general problematics of strongly correlated electronic systems. Beyond the low field (linear) conduction, the tunneling current-voltage J-U characteristics $J(U)$, $\sigma = dJ/dU$ are of particular importance. The interest has been renewed thanks to recently developed[2] design of intrinsic tunneling devices where electronic transitions between weakly coupled chains or planes take place in the bulk of the unperturbed material.

The first feature one expects to see at any tunneling experiment in gapful conductors is the regime of free electrons when the current onset corresponds to the voltage $U=E_g^0$ of the gap in the spectrum of electrons. But contrarily to usual systems, such as semiconductors or even superconductors, there is also a possibility for tunneling within the subgap region $E_g<U<E_g^0$. It is related to the pseudogap (PG) phenomenon known for strongly correlated electrons in general, well pronounces in quasi-1D systems and particularly in cases where the gap is opened by a spontaneous symmetry breaking (see Ref. 3, and references therein). The PG is originated by a difference, sometimes qualitative, between three forms of electronic states: (a) short living excitations which are close to free electrons, (b) dressed stationary excitations of the correlated systems, and (c) added particles which modify the ground state (g.s.) itself.[4] For our typical examples of electrons on a flexible lattice, the modification results in self-trapped states (b) such as single particle $\nu=1$ polarons with energies $W_1<\Delta_0$ below the single electron (a) activation energy Δ_0; then the new gap $E_g<E_g^0=2\Delta_0$ will be observed as a true threshold with the PG inbetween. There may also be contributions of two-particle $\nu=2$ states (c)—bipolarons, which energy gain per electron is larger than for polarons $W_2<2W_1$. While cases (a), (b) are common for low symmetry and discrete symmetry cases, for (c) there is a further drastic effect of a spontaneous symmetry breaking as in the case of the polyacethylene $(CH)_x$ or of some doubly commensurate charge density waves (CDWs). Now the bipolarons are decoupled into particles with a nontrivial topology, solitons or kinks, changing the sign of the order parameter of the dimerization. The situation is further intricate in systems with a continuous GS degeneracy similar to incommensurate charge density waves (ICDWs) or Wigner crystals. Here even the self-trapping of a single electron is allowed to lead to topologically nontrivial states, the amplitude solitons ASs. In the same class we find a more common case of acoustic polarons in a 1D semiconductor.[5,6]

Properties of systems with different types of g.s. degeneracy, and required theoretical approaches, are quite different. Here we shall concentrate on systems with a discrete, precisely double, degeneracy which also include most basic elements of nondegenerate systems. Theoretically, the tunneling in CDWs was studied in details for regimes of free electrons[7] when the current onset corresponds to the voltage $U=E_g^0$ of the gap in the spectrum of electrons. We shall consider the tunneling in the PG regime. We shall follow the method[3] developed for studies of single-particle spectral density $I(p,\omega)$ in applications to photoemission spectroscopy (PES) and angle-resolved PES (ARPES) intensities. We refer to this publication for details in techniques and literature.

A word on notations. In the following we shall invoke many quantities with the dimension of energy (or frequency, since we shall keep $\hbar=1$) which will be classified according to different characters (with indices). $U>0$ and $\Omega>0$ will be the external voltage difference for tunneling and the external frequency for PES or optics. $E>0$ will always stay for electronic eigenvalue in a given potential, negative values will be addressed explicitly as $-E$. $V_\nu(E)$ will be branches of a total energy (of deformations together with electronic energies) supporting eigenstates $\pm E$ which may be filled with occupation numbers $\nu=0$, 1, 2. W_ν will be total energies of stationary states, that is $W_\nu=\min_E V_\nu(E)=V_\nu(E_\nu)$. $\omega_0 \ll E$ will

be the frequency of a collective mode (phonons specifically to CDWs) which interaction with electrons is responsible for their self-trapping. The collective deformation $\Delta(x)$ will also be measured as the potential energy experienced by electrons. We shall keep the electron charge $e=1$ hence potentials will be measured as energies and the interchain current J will have the dimensions number of particles/unit time/unit length. The indices $j=a,b$ will number coupled chains; indices i will number moments τ_i of time for virtual processes.

II. SPECTROSCOPIES OF THE PSEUDOGAP

A possibility of tunneling or of other excitations within the gap in spectra of free electrons $E<\Delta_0$ is related to a more general phenomenon of the pseudogap PG. For electrons, the PG signifies the remnants of the spectral density $I(\Omega,P)$, or the integrated one $I(\Omega)=\int I(\Omega,P)dP/2\pi$, at $W_1<\Omega<\Delta_0$, where W_1 is the absolute boundary of the spectrum. W_1 is the energy of a fully dressed state of one electron interacting with other degrees of freedom. (There may be totally external modes such as deformations or polarizations for usual polarons, external modes essentially modified by the bath of electrons as in CDWs, internal collective modes of the electronic system itself as in SDWs.) Most commonly, the self-trapped state of one electron is known as the "polaron" while more complex objects, solitons, can appear for systems with continuously degenerate G.S.'s (see Ref. 8 for a review).

The functions $I(\Omega)$ and $I(\Omega,P)$ are measured directly in PES and ARPES experiments. As such they have been studied theoretically for the PG region by the present authors[3,5,6] and we refer to these publications for a more comprehensive discussion and review. The one electron spectra can also be accessed in traditional external tunneling experiments: junctions or scanning tunneling microscopy (STM). For the last case, and practically for macroscopic point junctions, only the integrated $I(\Omega)$ is measured. Elements of the full dependence $I(\Omega,P)$ become necessary to describe strongly anisotropic materials (layered quasi-2D or chain quasi-1D ones), where the coherent tunneling is realized in internal junctions of "mesa-type" devices.[2] Here the tunneling goes between adjacent layers within the single crystal of the same material, hence the momentum is preserved. In a simpler version, the internal subgap tunneling takes place from free electrons of some metallic bands or pockets to polaronic states within gapful spectra which probably takes place in $NbSe_3$.[9] Otherwise it measures actually the joint spectral density for creation a particle-hole excitation at adjacent chains (the interchain exciton). In this respect it will be instructive to compare the coherent tunneling and the subgap optical absorption (OA) (see a brief description and references in Ref. 3, Sec. III E). A less expected version of the internal tunneling is a possibility for bielectronic transfers (tunneling of bipolarons or of kink-antikink pairs) which is usually attributed only to superconductors. We shall see that these processes extend the PG further down to even lower voltages.

In any case, the tunneling current $J(U)$ is given by the transition rate of electrons between two subsystems a,b kept at the potential difference U. For a weak coupling $t_\perp$, the electron tunneling from a to b is given by the convolution of spectral densities

$$J \sim t_\perp^2 \int_0^U I_a(-\Omega,P) I_b(U-\Omega,P) |\Lambda(P)|^2 d\Omega dP$$

if the momentum is conserved, or of their integrals $J \sim t_\perp^2 \int_0^U I_a(-\Omega) I_b(U-\Omega) d\Omega$ for the incoherent tunneling. (Everywhere we assume $T=0$.) Recall that for free electrons with a spectrum $E(P)$ we have $I(\Omega,P) \sim \delta[|\Omega|-E(P)]$ while $I(\Omega)$ becomes the DOS $I(\Omega) \Rightarrow N(\Omega)$, e.g., for $D=1$ $I(\Omega) \sim t_\perp^2 m^{1/2} (\Omega-\Delta_0)^{-1/2}$ near the bottom of the free band where the electron effective mass is m.

Consider briefly the case where one of reservoirs, say b, is composed by free electrons with a known DOS $N_b(\Omega)$. One of applications of a tunneling between the free spectrum and the PG may be the case of several families of conjugated polymers (polypyrolle, polythiophene) where origins of filled, π or empty, π^* bands below and above the gap are essentially different. Then the polaronic effect, hence the PG, may be pronounced only for one type of particles: electrons or holes. The same concerns 1D systems made of semiconducting wires where both effective masses and deformation potentials for electrons and holes are usually very different. Then, for the incoherent tunneling, $I_a(U)$ gives directly either the tunneling current $J(U) \sim I_a(U)$ (if N_b has a sharp peak at the Fermi level, which is typical for using junctions with superconductors) or the tunneling differential conductance $\sigma = dJ/dU \sim I_a(U)$ (if $N_b \approx$ const at the Fermi surface).

Below we shall be mostly interested in systems with the charge conjugated symmetry (or qualitatively equivalent ones); the examples are carbon nanotubes, symmetric conjugated polymers such as polyphenylenes, polyanilines, and polymers where the gap is formed (partly at least) by the spontaneous symmetry breaking: the polyacethylenes.[10] Numerical details will be presented for the last rich case. In all these cases the PG will exist near both rimes $\pm\Delta_0$ of the free excitation gap $E_g^0=2\Delta_0$.

Recall now some known results for $I(\Omega)$ within the PG.[3] It has the form $I=A\exp(-S)$, where the action $S=S(\Omega)$ is proportional to the big parameter of our adiabatic approximation $S \sim \Delta_0/\omega_0 \gg 1$. $S(\Omega)$ is determined by an optimal fluctuation localized in space and time (an instanton) which supports the necessary split-off local level E. In principle, the prefactor $A=A(\Omega)$ also depends on Ω and may show power law dependencies near extremals $0, W_1$. But within constraints of the adiabatic approximation $\delta\Omega \gg \omega_0$ the dependence $A(\Omega)$ is negligible in comparison with the one of $S(\Omega)$. The characteristic value of A may be important for estimates of the overall magnitude of observable effects. Thus for the single particle integrated intensity $A \sim (\omega W_1)^{-1/2}$ and $A_P \sim (m\Delta_0 \omega W_1)^{-1/2}$ for the momentum resolved intensity; here m is the effective electron mass $m \sim \Delta_0/v_F^2$. Appendix B contains derivation of the prefactor specifically for the tunneling processes.

In limiting cases we have the following.[3]

(1) Near the entry to the PG, just below the free edge Δ_0:

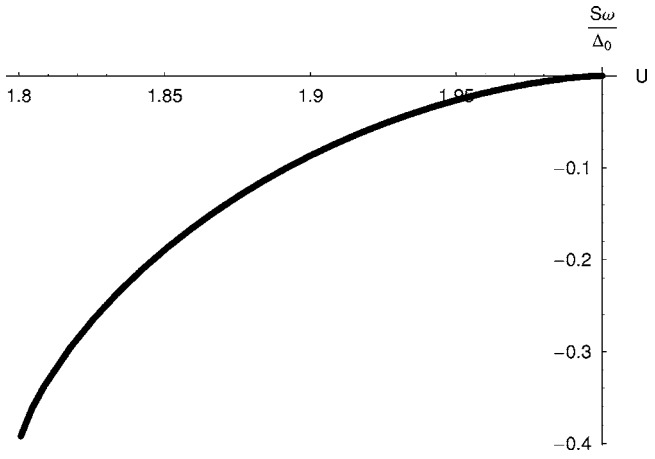

FIG. 1. The logarithmic plot for tunneling or absorption intensities $\ln I \sim -S$ in the pseudogap regime: between $2W_1$ and $2\Delta_0$.

$$\Delta_0 - W_1 \gg \Delta_0 - \Omega > 0\text{: } I = A \exp\left[- \frac{\text{const}}{\omega_0}\left(1 - \frac{\Omega}{\Delta_0}\right)^{3/2}\right]. \tag{1}$$

(2) Near the low end of the PG, just above the true spectral boundary W_1:

$$\Delta_0 - W_1 \gg \Omega - W_1 > 0\text{:}$$

$$I = A \exp\left[- \text{const}\frac{\Delta_0 - W_1}{\omega_0} - \text{const}\frac{\Omega - W_1}{\omega_0}\ln\left(\frac{\Omega - W_1}{\Delta_0 - W_1}\right)\right]. \tag{2}$$

The total dependence $I(\Omega)$ and the values of numerical constants in the above limiting laws, can be determined approximately[3] with the help of the instanton techniques simplified by the zero-dimensional reduction (the ansatz of an effective particle which we shall recall and extend below). The resulting curve is plotted in Fig. 1. Moreover, the regime 1 can be mapped exactly[3] upon the problem of a particle in a quenched random uncorrelated potential which here is created by instantaneous quantum fluctuations of the media. The known exact solution[11] provides the reference value of the coefficient in the exponent of Eq. (1), from which our approximate value differs only by 8%.[3]

Recall for comparison the usual regime $U > E_g^0$ of the allowed tunneling which is dominated by free electronic states. The current of the coherent tunneling between chains a,b is given as

$$J \sim t_\perp^2 \int \frac{dp}{2\pi}\delta[E_b(p) - U - E_a(p)]|\Lambda(p)|^2,$$

$$\Lambda(p) = \int dx \Psi_{bp}(x)\Psi_{ap}^*(x) \tag{3}$$

with $E_{a,b}(p) \approx \pm(\Delta_0 + p^2/2m_e)$ and $\Psi_{jp}(x)$ being the Bloch functions. It is instructive to compare the interchain tunneling probability with the on chain interband optical absorption OA when the matrix element of density $\Lambda(p)$ changes to the one of the momentum $t_\perp \Lambda(p) \Rightarrow \Lambda_{OA}(p)$. In both cases the e-h pair is created and the same spectral densities are involved. The difference is in matrix elements: the OA takes place between states of opposite parity while the tunneling requires for the same parity. The on-chain OA between edges $\pm\Delta_0$ of the free gap is known to be allowed since the parity of states near $\pm\Delta_0$ is opposite, hence Λ_{OA} is finite and the OA intensity as a function of frequency Ω rises as $I_{\mathrm{OA}} \propto 1/\sqrt{\Omega - 2\Delta_0}$. But for the same reason, the tunneling matrix element between identical chains is prohibited at $p=0$ and the tunneling will show only a weak edge onset $J \sim \sqrt{\Omega - 2\Delta_0}$. Nevertheless, in many cases of gaps opened due to spontaneous dimerization, the neighboring chains tend to order in antiphase. Now the shift by half a period permute states with $E \gtrless 0$ then the parity of states near opposite rims $\pm\Delta_0$ at neighboring chains is equal, the tunneling becomes allowed and the usual singularity is restored: $J \propto 1/\sqrt{U - 2\Delta_0}$.

Going down into the PG $\Omega < \Delta_0$, the above analysis applies to the on-chain optics but changes drastically for the interchain tunneling. The tunneling will be studied in detail below, here we shall only mention in advance an effect of spatial incoherence of optimal quantum fluctuations at different chains which removes completely the constraints of orthogonality. The case of the on-chain OA can be analyzed briefly already here. The OA is given by the convolution of two fast decaying functions of the energy

$$\begin{aligned} I_{\mathrm{OA}} &\sim \int I(\Omega_1, P) I(\Omega - \Omega_1, P)|\Lambda_{\mathrm{OA}}(P)|^2 d\Omega_1 dP \\ &\times \int \exp[-S(\Omega_1, P) - S(\Omega - \Omega_1, P)] \\ &\times |\Lambda(\Omega_1, \Omega_1 - \Omega)|^2 d\Omega_1 \\ &\sim \Lambda^2(\Omega/2, -\Omega/2)(S'')^{-1/2}\exp[-2S(\Omega/2)] \\ &= [S''(\Omega/2)]^{-1/2} I^2(\Omega/2); \quad S'' = \frac{d^2 S}{d\Omega^2}. \end{aligned} \tag{4}$$

Here we have used that for the convex function $S(\Omega)$, as given by Eqs. (1) and (2), the minimum of the expression $S(\Omega_1, P) + S(\Omega - \Omega_1, P)$ lies at the middle $\Omega_1 = U/2$. At this point the electron levels E and $E - \Omega$ are placed symmetrically, wave functions have opposite parity, hence $\Lambda(E, -E) \neq 0$ is finite. This is the case of typical Peierls insulators. But for systems where the basis wave functions of valent and conductive bands have the same parity (the dipole OA is not allowed), $\Lambda_{\mathrm{OA}}(E, -E) = 0$ and we have to consider in Eq. (4) the deviations from the symmetry condition. Now $\Lambda_{\mathrm{OA}}(E_a, E_b) \sim (E_a + E_b)^2$ and the saddle point integration in Eq. (4) gives another factor of $1/S''$ which is small as $\sim \omega_0/\Delta_0$. We arrive at the answer similar to Eq. (4) but with the small prefactor $(S'')^{-3/2}$.

Until now we did not consider the dependencies on the momentum P. In the full range of Ω and P, the spectral function $I(\Omega, P)$ has a rich structure which can be tested in the ARPES experiments. In observable quantities, the momentum dependence appears twice: via the matrix element

$\Lambda(P)$ and via the action $S(\Omega) \Rightarrow S(\Omega, P)$. The analysis is simplified for the regime 2: the low polaron boundary W_1. Here the action dependence on Ω and P comes through the single variable $\Omega \Rightarrow \Omega + P^2/2M_1$, where $M_1 \sim m\Delta_0^2/\omega_0^2$, is a heavy mass of the polaron center motion. This kinetic energy contribution can be neglected in comparison to the matrix element dependence on P which confines $\Lambda^2 \sim |\Psi_P|^4$ within the characteristic momenta distribution $|\Psi_P|^2$ of the wave function $\Psi(x)$ of the self-trapped electronic state localized over the scale $L \sim \xi_0$: beyond $P \sim \xi_0^{-1} = \Delta_0/\hbar v_F$, the function $\Lambda(P)$ falls off exponentially. (At this scale, the recoil kinetic energy $P^2/2M \sim \omega_0^2/\Delta_0$ is small in comparison with the energy width $\epsilon \sim (S'')^{-1/2} \sim [\omega_0(W_1 - \Omega)]^{1/2} \gg \omega_0$. Then the final integration over P affects only $\Lambda(P)$ and gives a constant factor $\sim 1/\xi_0$.) Altogether we find for tunneling the law (2) with $\Omega \to U/2$.

In the regime 1, near the free edge, the states are shallow $\epsilon = 1 - E/\Delta_0 \ll 1$ and extended $L/\xi_0 \sim \epsilon^{-1/2} \gg 1$. The effective mass M for the center-of-motion becomes slightly energy dependent

$$M \sim \frac{\epsilon^2}{\omega_0^2 L} \sim \frac{\epsilon^{5/2}}{\omega_0^2},$$

but the characteristic energy scale of the form factor $\sim M^{-1}L^{-2} \sim \omega_0^2 \epsilon^{-3/2}$ is still small in comparison with the characteristic energy width $\sim \omega_0^{2/3}$ of Eq. (1). So again we integrate separately the factor $\int \Lambda^2(P) dP \sim \int dP \Psi_P^4 \sim L$ to obtain an additional prefactor $\epsilon^{-1/2}$ for the tunneling law (1) with $\Omega \to U/2$.

Recall that for the ARPES with independent variations of Ω and P, their interference may lead to rather unexpected and potentially observable phenomena (Ref. 3, Sec. III D). One of them is the "quasispectrum:" the intensity maximum over the line $\Delta_0 - \Omega \sim P^{1/2}$ within the PG $\Omega < \Delta_0$ [Ref. 3, Sec. III D, case B1, Eq. (49)]. Another effect is the emergence of instantons at high P within the domain of free electron region $> \Omega > \Delta_0$ leading to the enhanced intensity within the band $0 < \Omega - \Delta_0 < \text{const}/P^3$ [Ref. 3, Sec. III D, case B3, Eq. (51)].

III. TUNNELING: THE DERIVATIONS

We shall follow the adiabatic method of earlier publications[3,5,6] assuming a smallness of collective frequencies ω_0 in compare with the electronic gap $\omega_0 \ll \Delta_0$. Now, electrons are moving in a slowly varying potential $\Delta(x,t)$, so that at any instance t their energies $E_j(t)$ and wave functions $\Psi_j(x,t)$ are defined from a stationary Schrodinger equation $H\Psi(x,t) = E(t)\Psi[x,E(t)]$ [Eq. (A1) below will give an example]. The Hamiltonian $H = H[x, \Delta(x,t)]$ depends on the instantaneous configuration $\Delta(x,t)$ so that $E(t)$ and $\Psi[x,E(t)]$ depend on time only parametrically. Exponentially small probabilities which we are studying here are determined by steepest descent paths in the joint space $[\Delta(x), t]$ of configurations and the time, that is by a proximity of the saddle point of the action S. It is commonly believed, in analogy with the usual WKB, that the saddle point, the extremum of S over Δ and t, lie at the imaginary axis of t so that, as usual, we shall assume $t \Rightarrow it$ and correspondingly $S \Rightarrow iS$ since now on.

Consider the system of two weakly coupled chains $j = a, b$ which are put at the electric potential difference U. The system is described by the total action

$$S_{ab} = S_a + S_b + t_\perp \int dxdt[\hat{\Psi}_a^\dagger(x,t)\hat{\Psi}_b(x,t) + \hat{\Psi}_b^\dagger(x,t)\hat{\Psi}_a(x,t)], \tag{5}$$

where $S_j = S[\Delta_j(x,t)]$ are single chain actions and the term $\sim t_\perp$ describes the interchain hybridization of electronic sates. $\hat{\Psi}_j(x)$ are operators of electronic states. The average transverse current is given by the functional integral

$$J = \frac{\int D[\Delta_j(x,t)] i t_\perp [\hat{\Psi}_a^\dagger(x,t)\hat{\Psi}_b(x,t) - \hat{\Psi}_b^\dagger(x,t)\hat{\Psi}_a(x,t)] \exp[-S_{ab}]}{\int dx D[\Delta_j(x,t)] \exp[-S_{ab}]}. \tag{6}$$

A. One electron tunneling

We consider first the processes originated by the transfer of one electron between the chains. They appear already in the first order of expansion of the exponent in Eq. (5) in powers of $t_\perp$, which contribution to the current (6) can be written as

$$J = Z_0^{-2} t_\perp^2 \int D[\Delta_j(x,t)] \int d(x-y) \int d(\tau_1 - \tau_2) (\Psi_a^*(x,\tau_1)\Psi_b(x,\tau_1)\Psi_a(y,\tau_2)\Psi_b^*(y,\tau_2) \exp\{-S[\tau_1 - \tau_2, \Delta_j(x,t)]\}), \tag{7}$$

where the normalizing factor Z_0^{-2} is the denominator in Eq. (6) taken at $t_\perp = 0$. Here the time dependent action $S(\tau_1 - \tau_2)$ describes (in imaginary time) the process of transferring one particle from the doubly occupied level $E_a < 0$ of the chains a to the unoccupied level $E_b > 0$ of the chain b at the time τ_1 and the inverse process at the time τ_2. We have

$$S[\tau_1-\tau_2,\Delta_j(x,t)]=\left\{\int_{-\infty}^{\tau_1}+\int_{\tau_2}^{\infty}\right\}dt[L_a(0)+L_b(0)]+\int_{\tau_1}^{\tau_2}dt[L_a(-1)+L_b(1)-U]=\int_{-\infty}^{\infty}dt[L_a(0)+L_b(0)]+\int_{\tau_1}^{\tau_2}dt(E_b+E_a-U), \quad (8)$$

where $L_j(\nu)=L([\Delta_j],\nu)$ are Lagrangians of the jth chain with the number of electrons changed by ν. They are given as a sum of the kinetic term and the potential V_ν:

$$L_j(\nu)=\int dx\frac{(\partial_t\Delta)^2}{g^2\omega_0^2}+V_\nu[\Delta(x,t)];\quad V_\nu=V_0+|\nu|E. \quad (9)$$

Here the potential term V_ν contains the energy of deformations and the sum over electron energies in filled states α which include both the vacuum states and the split off ones

$$V_\nu[\Delta(x,t)]=\int dx\frac{\Delta^2}{2g^2}+\sum_{E_\alpha<E_F}E_\alpha[\Delta(x,t)]-W_{\text{g.s.}} \quad (10)$$

(here g is the coupling constant). V_ν is counted with respect to the g.s. energy $W_{\text{g.s.}}$ so that in the nonperturbed $\Delta\equiv\Delta_0$ state $V_\nu=|\nu|\Delta_0$ (the particle, electron for $\nu>0$ or hole for $\nu<0$, added instantaneously to the nondeformed g.s. is placed at the lowest allowed energy, the gap rim Δ_0).

The exact extremal (saddle point) trajectory is defined by equations

$$\delta S/\delta\Delta_j(x,t)=0,\quad \partial S/\partial\tau_1=\partial S/\partial\tau_2=0. \quad (11)$$

Actually the explicit calculation of the action requires for approximations. We shall follow a way[3] of the zero-dimensional reduction which reduces the whole manyfold of functions $\Delta_j(x,t)$ to a particular class

$$\Delta_j(x,t)\Rightarrow\Delta_E[x-X_j(t),E_j(t)],\quad S[\Delta_j(x,t)]\Rightarrow S[E_j(t),X_j(t)] \quad (12)$$

of a given function Δ_E of x [relative to a time-dependent center-of-mass coordinate $X_j(t)$]. $\Delta(x)$ is parameterized by a conveniently chosen (see Ref. 3 for examples) parameter for which a universal and economic choice is the eigenvalue $E_j(t)$. The requirement for the manyfold $\Delta(x,E)$ is that it supports a pair of eigenvalues $\pm E$ split off inside the gap $(-\Delta_0,\Delta_0)$ which span the whole necessary interval. The last simplification is to assume, in the spirit of all approaches of optimal fluctuations,[12,13] that the potential supports one and only one pair of localized eigenstates $\Psi(x,\pm E)$. Explicit formulas for the Peierls case are given in Appendix A.

Recall that for the OA problem we deal with one chain characterized by one pair of functions $E(t)$ and $X(t)$. But for the interchain tunneling, the functions $E_j(t)$ at chains $j=a,b$ are not obliged to be identical and also the wells may be centered around different points $X_j(t)$. Within such a parametrization the variational equation in Eq. (11) yields the equation of motion for $E(t)$

$$f(E_j)\left(\frac{dE_j}{dt}\right)^2-V_\nu(E_j)-|\nu|U+H_{\nu j}=0,$$

$$f(E)=\frac{1}{g^2\omega_0^2}\int dx\left(\frac{\partial\Delta(x,E)}{\partial E}\right)^2, \quad (13)$$

where $H_{\nu j}=$const are the Hamiltonians which must be constants within each interval of integration in Eq. (8). Apparently, at the outer intervals ($t<\tau_1$), ($\tau_2<t$) $H_{0j}=0$ to provide the return to the g.s. with $V_0=0$ at $t\to\pm\infty$. At the inner interval ($\tau_1<t<\tau_2$) $H_{1j}=E_j(\tau_1)+U=E_j(\tau_2)+U$ to preserve the continuity of velocities $\dot{E}_j$ at $t=\tau_{1,2}$. Since the values $E_j(\tau_{1,2})$ are determined uniquely by the equation of motion at the outer intervals, then $E_j(\tau_{1,2})$ coincide for both $j=a,b$, hence $H_a=H_b$ and the functions $E_j(t)$ become identical at any time $E_a(t)\equiv E_b(t)\equiv E(t)$. [Still, the shapes are allowed to be shifted by different centers $X_j(t)$: $\Delta_a(x-X_a,t)\equiv\Delta_b(x-X_b,t)$]. Finally the extremal conditions (11) with respect to impact times τ_i in Eq. (8) yield

$$E_a(t)+E_b(t)_{t=\tau_{1,2}}=U\quad\text{hence } E_a(\tau_{1,2})=E_b(\tau_{1,2})=U/2.$$

The action is finite $S<\infty$, hence the transition probability is not zero, only for a closed trajectory, that is at presence of a turning point (as examples, see Figs. 5–8 in Appendix A). There must be a minimal value of $E=E_m$ where $\dot{E}=0$ hence $V_1(E_m)=U/2$ and $E_m<U/2$. The last condition requires for $\min V_1(E)=W_1\leqslant U/2$ that is for $U>2W_1$ which determines the threshold voltage at twice the polaron energy.

We arrive at the effective one chain problem with the doubled effective action. The extremal tunneling action is $S_{\text{tun}}=2S_I$ which is twice the exponent appearing in the spectral density I with limiting laws (1) and (2). The full expression is

$$S_{\text{tun}}(U)=8\int_{E_m}^{U/2}dE\sqrt{f(V_1-U/2)}+8\int_{U/2}^{\Delta_0}dE\sqrt{fV_0};\quad V_1(E_m)=U. \quad (14)$$

We obtain a final expression for the current after integration over $\Delta_j(x,t)$ around the extremal taking into account the zero modes related with translations of the instanton center positions $X_j(t)$ (details of calculations are given in Appendix B)

$$J(U)\propto t_\perp^2M_U\omega_0\sqrt{\frac{dT}{dU}}\int\frac{dp}{2\pi}e^{-p^2l^2/4}|\Psi_p(U/2)\Psi_p(-U/2)|^2\times\exp[-2S_I(U/2)], \quad (15)$$

where Ψ_p is the Fourier transforms of the wave functions $\Psi(x)$ and time T is defined as $T=\int_{U/2}^{E_m}dE/\dot{E}$. The mean fluctuational displacement l of the center of mass between the impact moments is given as

$$l^2 = \int_{\tau_1}^{\tau_2} \frac{dt}{M[E(t)]} = 2\int_{E_m}^{U/2} \frac{dE}{M(E)} \frac{\sqrt{f(E)}}{\sqrt{V_1(E) - U/2}},$$

where $M(E)$ is the translational mass:

$$M(E) = \frac{2}{g^2\omega_0^2} \int dx \left(\frac{\partial \Delta(x,E)}{\partial x} \right)^2, \quad M_U = M(U/2). \quad (16)$$

Note that the prefactor in Eq. (15), which is the matrix element between orthogonal states $\Psi(E)$ and $\Psi(-E)$, is always nonzero due to the integration over zero modes $X_j(t)$ (in contrast to results for the rigid lattice where it obeys the selection rules); see more in Appendix B.

Comparing with the PES intensity $I(\Omega)$ calculated in Ref. 3 we see that, up to preexponential factors, the tunneling current is proportional to the square of the PES intensity I: $J \propto t_\perp^2 I^2(\Omega = U/2)$. For example, near the threshold $U = 2W_1$ we can write

$$J \sim \frac{t_\perp^2}{\Delta_0 \xi_0} \left(\frac{\Delta_0}{\omega_0} \right)^{3/2} \exp\left[-C_1 \frac{\Delta_0}{g\omega_0} \right] \times \exp\left[C_2 \frac{(U - 2W_1)}{g\omega_0} \ln \frac{2C_3\Delta_0}{(U - 2W_1)} \right]. \quad (17)$$

The coefficients $C_i \sim 1$ can be found numerically from Eq. (14) as (for the Peierls model) $C_1 = 0.4$, $C_2 = 2.9$, $C_3 = 0.1$. (These values differ from the corresponding ones in Ref. 3 because of different normalizations of frequency ω_0 in compare to $\omega_{\rm ph}$.)

B. Bielectronic tunneling

It is known that the joint self-trapping of two electrons allows one to further gain the energy resulting in stable states different from independent polarons. In general nondegenerate systems this is the bipolaron, confined within the length scale twice smaller than that of the polaron, the energy gain of the bound state $\delta E = \Delta_0 - E$ is four times that of the polaron and the total energy gain of the bipolaron $\delta W_2 = 2\Delta_0 - W_2$ is also four times that of two polarons. (Certainly these results neglect the energy loss due to the Coulomb repulsion which may become critical for the stability of a shallow bipolaron.) At the same time, the total energy of one bipolaron $W_2 = 2\Delta_0 - \delta W_2$ is larger than the energy of one polaron $W_1 = \Delta_0 - \delta W_1$ and even than the free electron energy Δ_0. This is why bipolarons cannot be seen as thermal excitations while they are favored in case of doping. The information on their existence comes from the ground state of doped systems where bipolarons are recognized by their spinless character and special optical features (see Ref. 14 for experimental examples on conducting polymers and Ref. 15 for relevant theoretical models). An important advantage of tunneling experiments is a possibility to see bipolarons directly, at voltages U below the two-polaron threshold $2W_1$ which is within the true single particle gap. This possibility comes from the fact that, for bipolarons as particles with the double charge $2e$, the voltage gain by transferring from one chain to another is $2U$, hence the threshold will be at $U = W_2 < 2W_1$. The probability of the bielectron tunneling is small as it appears only in the higher order $\sim t_\perp^4$ in interchain coupling. But it can be seen as extending below the one-electron threshold where no other excitations can contribute to the tunneling current.

The bielectronic contribution to the current can be written, by expanding Eqs. (5) and (6) as

$$J_2 = Z_0^{-2} t_\perp^4 \int D[\Delta_a] D[\Delta_b] \int \prod_{i=1}^{3} dy_i d\tau_i \exp[-S(\tau_i)] \times [\Psi_a^*(x,\tau)\Psi_b(x,\tau)\Psi_a^*(y_1,\tau_1)\Psi_b(y_1,\tau_1)\Psi_b^*(y_b,\tau_2) \times \Psi_a(y_2,\tau_2)\Psi_b^*(y_3,\tau_3)\Psi_a(y_3,\tau_3) - \{2 \leftrightarrow 3\}],$$

which generalizes expressions (7) and (8) for the electron one tunneling. Here

$$S(\{\tau_i\}) = \left\{ \int_{-\infty}^{\tau} + \int_{\tau_3}^{\infty} \right\} dt[L_a(0) + L_b(0)] + \left\{ \int_{\tau}^{\tau_1} + \int_{\tau_2}^{\tau_3} \right\} \times dt[(L_a(1) + L_b(1) - U] + \int_{\tau_1}^{\tau_2} dt[L_a(2) + L_b(2) - 2U]. \quad (18)$$

Within our model (9) and (10) the potentials V are additive in energy E, then the action can be simplified as

$$S(\{\tau_i\}) = 2\int_{-\infty}^{\infty} dt L_a(0,t) + \left\{ \int_{\tau}^{\tau_1} + \int_{\tau_2}^{\tau_3} \right\} \times dt[E_a(t) + E_b(t) - U] + 2\int_{\tau_1}^{\tau_2} dt[E_a(t) + E_b(t) - U]. \quad (19)$$

The extremal solution is defined, as above, by equations of the type (11) but with four impact times τ_i instead of two. (Actually, in view of the time reversion symmetry, the number of boundary conditions is twice smaller.) A similar analysis of the extremal solution shows that optimal fluctuations $\Delta_j(x,t)$ are identical in shape, up to shifts of their centra: $X_j(t)$, $\Delta_j(x,t) \equiv \Delta(x - X_j, t)$. Hence the energies are identical $E_a(t) \equiv E_b(t)$, and also the resonance conditions $2E(\tau_i) = U$ take place at the impact moments τ_i. Moreover, the simple hierarchy of our model $V_2 - V_1 \equiv V_1 - V_0 \equiv E - U/2$ shows that all branches $V_\nu(E)$ cross at the same point $E = U/2$ (see Figs. 5–7 below). Then the evolution $E(t)$ switches directly from the branch $\nu = 0$ to the branch $\nu = 2$ and back, without following the intermediate branch $\nu = 1$. It means that the intervals (τ, τ_1) and (τ_2, τ_3) of one-electron transfers $\nu = 1$ are confined to zero: $\tau = \tau_1$, $\tau_2 = \tau_3$. In other words, only processes of simultaneous tunneling of pairs of particles are left. Notice that this picture changes in more general models, particularly taking into account important Coulomb interactions. They add, to the energy branch of a shallow bipolaron, the energy $\delta V_2 \sim (e^2/\epsilon_\perp L)\ln(L/a_\perp)$, where $\epsilon_\perp$ is the dielectric susceptibility of the media in the interchain direction, $L = L(E)$ is the localization length of $\Psi(x,E)$, such that $E \sim 1/(mL^2)$. Now the intermediate intervals $(\tau = \tau_1), (\tau_2 = \tau_3)$ appear where the evolution follows the $\nu = 1$ branches, see Fig. 8. With increasing Coulomb interactions this single par-

ticle interval becomes more pronounced and the bipolaronic threshold is shifted towards the one of two independent polarons.

In any case, the extremum solution for the action (18) is achieved on the instanton trajectory given be the equation

$$f(E)\dot{E}^2 = V_U(E) = \min\{V_0(E), V_1(E) - U/2, V_2(E) - U\}.$$

The extremal action is

$$S_2(U) = 8\int_{E_m}^{\Delta_0} dE\sqrt{f(E)V_U(E)}; \quad V_U(E_m) = V_2(E_m) - U = 0. \tag{20}$$

This action is finite if the turning point E_m does exist, that is if $U \geqslant \min V_2 = W_2$.

Notice that, neglecting Coulomb interactions, the energy V_ν is determined only by the total number $\nu = \nu_e + \nu_h = \nu(E) + [2 - \nu(-E)]$ of electrons and holes. Then the energy of the bipolaron [both $\nu(E)$ and $\nu(-E)$ are either empty or doubly occupied] and the energy of the exciton [both $\nu(E)=1$ and $\nu(-E)=1$ are singly occupied] are the same. Then the trajectory of the bielectronic tunneling becomes the same as the one for the case of optical absorption,[3] only the action is doubled $S_2(U) = 2S_{\mathrm{OA}}$ $(\Omega = U)$. Up to the preexponential factor we have

$$J_2 \propto t_\perp^4 [I_{\mathrm{OA}}(\Omega = U)]^2, \tag{21}$$

where $I_{\mathrm{OA}}(\Omega)$ is the optical absorption probability for one chain.

For common systems with a nondegenerate ground state, the dependence $S_2(U)$ resembles qualitatively the law (17) for the one-electron contribution, with a similar behavior near the threshold $U - 2W_1 \to U - W_2$. The situation changes for a doubly degenerate ground state where the bipolaron dissolves into a diverging pair of solitons (dimerization kinks). Thus for the Peierls model the evaluation of Eq. (20) gives, similar to the OA law of Ref. 3, near the two particle threshold

$$J_2 \sim t_\perp^4 \exp\left(-\max S_2 + \frac{4}{g\omega_0}\sqrt{6\Delta_0(U - 2W_s)}\right);$$
$$\max S_2 = C_4\Delta_0/g\omega_0 \tag{22}$$

with $C_4 = 3.77$. The overall dependence for the $\ln J_2(U) \sim -S_2(U)$ is shown in Fig. 2. Here we see explicitly that in the order $\sim t_\perp^4$ the threshold voltage $U = 2W_s$ is smaller than $U = 2W_p$ obtained in the order $\sim t_\perp^2$. Therefore this is the main contribution to the current in the region $2W_s < U < 2W_p$. Figure 2 shows that the dependence of $J_2(U)$ near the low U onset is much sharper than that of $J(U)$ in Fig. 1 near the polaronic onset which corresponds to the higher singularity in the limiting formula (22) in comparison to Eq. (17).

IV. DISCUSSION AND CONCLUSIONS

In quasi-1D systems with a gapful electronic spectrum, the interchain tunneling (as well as PES or OA) can be used to test virtual electronic states within the pseudogap. Due to

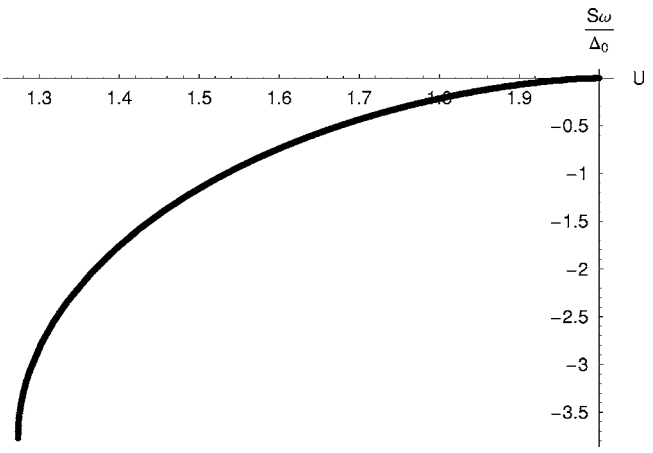

FIG. 2. The logarithmic plot for bielectron tunneling or for optical absorption intensities $\ln I \sim -S$ in the two particle pseudogap regime: between $2W_s$ and $2\Delta_0$. Notice the $\sqrt{\Omega - 2E_s}$ singularity near the two soliton threshold.

the interaction of electrons with a low frequency mode, phonons in our examples, the tunneling is allowed in the subgap region $U < E_g^0$ which forms the pseudogap. The one electron processes lead to universal results similar both for systems with the build-in gap and for those where the gap is due to the spontaneous breaking of a discrete symmetry. The PG is entered with the law (1) and continues down to the threshold $U_1 = 2W_1$, approached with the law (2). This threshold corresponds to the interchain transfer of fully dressed particles: polarons with the energies W_1. But in tunneling the PG is stretched even further down thanks to processes of a simultaneous tunneling of two electrons. It terminates at the lower threshold $U_2 = W_2$ or $U_2 = 2W_s$, $U_2 < U_1$. Here W_2 is the energy of the bipolaron—a bound state of two electrons self-trapped together. In degenerate systems the bipolaron dissolves into unbound solitons, hence the threshold at $2W_s$ with a more pronounced dependence of the tunneling rate (22) as well of the OA. Numerical results are presented in Figs. 1 and 2.

There is an important difference between subgap processes and the usual overgap transitions at $U, \Omega > E_g^0$ of free electrons in a rigid system. It comes, beyond intensities, from different character of matrix elements. Actually within the PG region there are no particular selection rules since the wave functions of virtual electronic states split off within the gap are localized having a broad distribution of momenta. Then the PG absorption is allowed independent on the interchain ordering. Contrarily, the regular tunneling across the free gap shows an expected DOS singularity $\sim (E - E_g^0)^{-1/2}$ for the out of phase interchain order while for the in-phase order the threshold is smooth $\sim (E - E_g^0)^{1/2}$. This difference may be important to choose an experimental system adequate for studies of PGs. The smearing of the free edge singularity is a natural criterium for existence of the PG below it.[16] But the total absence of this strong feature in systems with forbidden overgap transitions can allow for a better resolution of the whole PG region, down to the absolute threshold. Probably a very smooth manifestation of gaps in usual tunneling experiments on CDWs,[17] while the gaps

show up clearly through activation laws, is related to this smooth crossover from the overgap to the subgap region. (Notice that the existing experiments refer mostly to ICDWs which, with their continuous degeneracy of the GS, must be studied specially which is beyond the scope of this article.)

Finally we shall discuss relations with other theoretical approaches. Most theories of tunneling, see Ref. 7, keep the following assumptions. (i) They refer to the overgap region where interactions or fluctuations are not important and usually are not taken into account. (ii) They refer to the incoherent tunneling, local in space, which is a usual circumstance of traditional experiments. The PG in tunneling was considered by Monz *et al.* in Ref. 7 in the framework of the approach.[18] This method became popular recently in theories of the PG thanks to its easy implementation: it is sufficient to average results for a rigid system over a certain distribution of the gap values. Apparently this is the way to describe an average over a set of measurements performed on similar systems with various values of the gap, e.g., manipulating with the temperature, the pressure or a composition. But actually, as we could see above, the PG is formed by fluctuations localized both in space and time, the instantons, with localization parameters depend on the energy deficit being tested. There is an intermediate approach applied[19] to a complex of the PG phenomenon from optics to conductivity and susceptibility. It treats fluctuations as an instantaneous disorder due to quantum zero point fluctuations of the gap. Indeed, this picture can be well applied, as it was done already in Ref. 20, but only to dynamical processes and only in the upper PG region, just below the free gap E_g^0, which leads to the law (1). But deeper within the PG, the fluctuations are not instantaneous: they require for an increasingly longer time and become self-consistent with the measured electronic state leading to another law and to appearance of the lower threshold. Generalizations and deeper analysis of the model of the instantaneous disorder lead to interesting theoretical studies,[21] but their applicability is very limited unless the variable time scale is realized as we have demonstrated in this and preceding articles.

Our approach can be compared to the work[22] on the fluctuational creation of pairs of phase solitons in a 1D commensurate CDW under the longitudinal electric field. But in our case we deal, in effect, with the interchain tunneling of pairs of solitons under the transverse field; also the solitons have a more complex character of a multielectronic origin.

In conclusion, the presented and earlier[3,5,6] studies recall for the necessity of realizing the variable time scale of subgap processes both in theory and in diverse interpretations of different groups of experiments (dynamic, kinetic, thermodynamic) which address excitations with very different lifetimes.

ACKNOWLEDGMENTS

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APPENDIX A: DETAILS ON SELF-TRAPPING BRANCHES

We consider the system of weakly coupled dimerized chains. Each chain is described by a usual electron-phonon Hamiltonian (Peierls, SSH models). Electron levels E and wave functions $\Psi=\Psi(x,E)$ are determined by equations

$$[-v_F i\partial_x\sigma_3+\Delta(x)\sigma_1]\mathbf{\Psi}=E\mathbf{\Psi}, \tag{A1}$$

where $\sigma_{1,3}$ are the Pauli matrices $\mathbf{\Psi}=(\Psi_+,\Psi_-)$, $\Psi_\pm(x)$ are the components of electron wave functions near Fermi points $\pm p_F$, and the real function $\Delta(x)$ is the amplitude of the alternating dimerization potential. The ground state of each chain is the Peierls dielectric with the gap $2\Delta_0$. The electron spectrum has the form $E_p^2=v_F^2p^2+\Delta_0^2$ (in the following we shall put the Fermi velocity $v_F=1$, $\Delta_0=1$ and, as everywhere, the Plank constant $\hbar=1$). The excited states are solitons (kinks), polarons and bisolitons (kink-antikink pairs) which are characterized by electron levels localized deeply within the gap (see Ref. 8). The one parametric family of configurations $\Delta(x,E)$ supporting the single split-off pair of levels $\pm E$ can be written as

$$\Delta(x,E)=1-\frac{2(1-E^2)}{1+E\cosh[2x(1-E^2)^{1/2}]} \tag{A2}$$

evolving from a shallow potential well at $E\approx 1$ through the stationary configuration for a polaron $\nu=1$ to the pair of diverging kinks at $E\to 0$ as shown in Fig. 3. The potentials V_ν (for the E level filling ν) as functions of E are given as

$$V_\nu(E)=\nu E+\frac{4}{\pi}\sqrt{1-E^2}-\frac{4}{\pi}E\cos^{-1}E. \tag{A3}$$

The translational mass can be found as

$$M(E)=\frac{8\Delta_0^3}{g^2\omega_0^2}\left[\frac{1}{3}\tan^3\left(\cosh^{-1}\frac{1}{E}\right)-E^2\cosh^{-1}\frac{1}{E}+E^2\sqrt{1-E^2}\right]. \tag{A4}$$

Consider the matrix element between levels $\pm E$ in the Peierls state. The wave function has two components (u,w) according to $\Psi=\Psi(x,E)=u\cos p_Fx+w\sin p_Fx$. Explicit expressions for split-off states are $u,w\sim\sqrt{1-\Delta^2}\pm\partial_x\Delta$. The equation for the bound eigenstate (A1) shows the following symmetry: $w(x,E)=u(-x,E)$, $w(x,-E)=u(x,E)$, $u(x,-E)=-u(-x,E)$. Then $\Psi(x,E)=[(u(x),u(-x))]$, $\Psi(x,-E)=[-u(-x),u(x)]$, with $u=u(x,E)$, which explicitly demonstrates the orthogonality of $\Psi(x,E)$ and $\Psi(x,-E)$. The matrix element in Eq. (15) becomes $\Lambda_p^2\sim|\Psi_p(E)\Psi_p(-E)|^2=|-u_pu_{-p}+u_pu_p|^2$. At $p=0$, $\Lambda=\Lambda_0=0$, hence for identical chains the transition at the free gap $\Omega=2\Delta_0$ is forbidden which removes the singularity at the gap threshold in a rigid system. But the true threshold at $2W_1$ for the subgap absorption or tunneling are not subjected to this selection rule since the wave functions of localized states associated to the optimal fluctuation are distributed over the momentum region $p\sim\xi_0^{-1}$.

Figure 3 shows the exact shapes $\Delta(x,E)$ of the equilibrium polaron (upper thick line) and of a well formed ($E=0.01$) pair of solitons (lower thick line). Thin lines show exact shapes of optimal fluctuations necessary to create these states by tunneling. Notice the much less pronounced shapes for optimal fluctuations in compare to the final states which facilitates the tunneling.

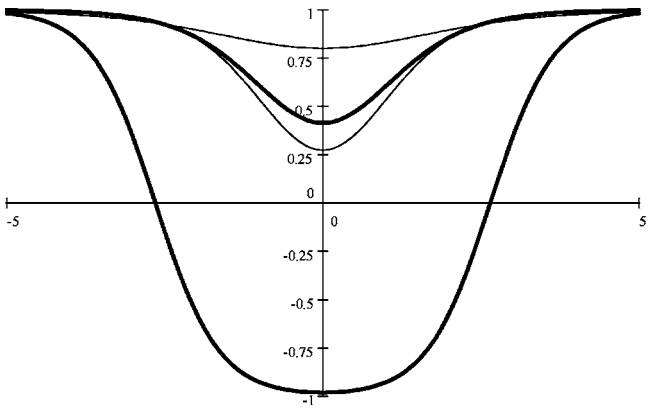

FIG. 3. Exact shapes $\Delta(x,E)$ of the equilibrium polaron $E=2^{-1/2}$ (upper thick line) and of a nearly formed ($E=0.01$) pair of solitons (lower thick line). Thin lines show exact shapes of optimal fluctuations necessary to create these states by tunneling.

Figure 4 plots the total energy $V_1(E)$ of the single particle branch as a function of the associated energy of the bound state. $E=1$, $V_1(1)=1$ corresponds to the particle added to the unperturbed ground state, at the bottom of the continuous spectrum. $E=0$ is the midgap state reached for the limit of two divergent solitons when the total energy approaches the maximal value $V_1(0)=2W_s=4/\pi\approx 1.27$. In between, at $E_1=2^{-1/2}\approx 0.7$, $V_1(2^{-1/2})=W_1=2^{3/2}/\pi\approx 0.9$, the minimum corresponds to the stationary polaronic state. The short thin vertical line between plots E and $V_1(E)$ points to the configuration (upper thin curve at the top of Fig. 3) of the fluctuation necessary for tunneling to the polaron [the minimum of $V_1(E)$, upper thick curve in Fig. 3].

The next three figures plot the total energies $V_\nu-\nu U$ for different branches as a function of the energy E of the associated bound state (all in units of Δ_0). Branches are distinguished by their ordering at $E=1$. Figure 5 corresponds to the potential $U=1.2$ which is below the bielectronic threshold; no branch is crossing $V=0$ axis, hence no final action is allowed and the current is zero.

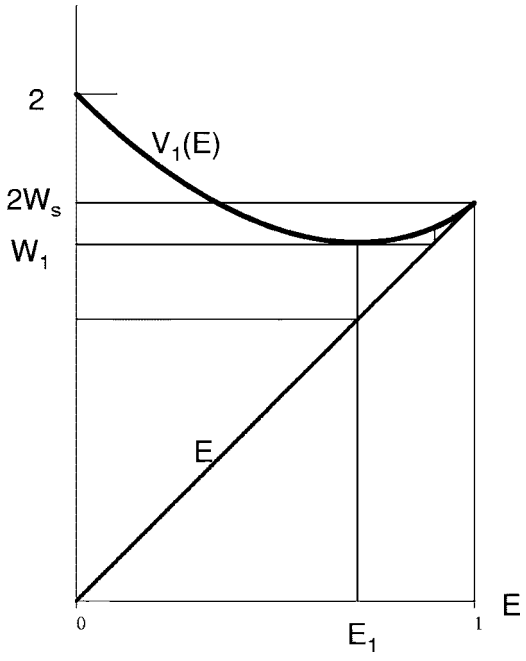

FIG. 4. Total energy of the single particle branch $V_1(E)$ as a function of the energy E of the associated bound state.

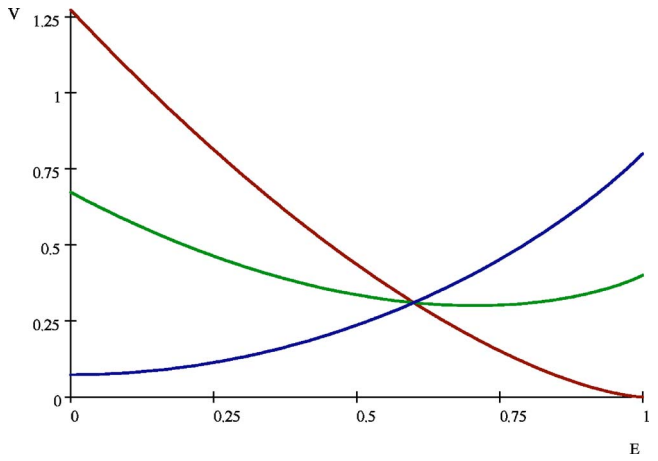

FIG. 5. (Color online) Total energies $V_\nu-\nu U$ for different tunneling branches $V_\nu-\nu U$ as a function of the energy E of the associated bound state. This figure corresponds to $U=1.2$ which is below the bielectronic threshold.

Figure 6 corresponds to the potential $U=1.4$ which is between the bielectronic threshold $2W_s=4/\pi\approx 1.3$ and the polaronic one $2W_1=1.8$; the bielectronic branch crosses the axis $V=0$ at the point E_m, the action is finite, hence a nonzero tunneling of two electrons is allowed.

Figure 7 corresponds to the potential $U=1.8$, above the bielectronic threshold $2W_s=4/\pi\approx 1.3$, exactly at the polaronic one $2W_1=1.8$. Now two parallel processes of one- and two-electron tunneling are allowed.

Figure 8 corresponds to the potential $U=1.6$ between the bielectronic threshold $2W_s=4/\pi\approx 1.3$, and the polaronic one $2W_1=1.8$. Contrary to Fig. 6, the Coulomb interaction is taken into account which lifts the degeneracy of the earlier crossing point of three branches. The one electron term $\nu=1$ does not cross $V=0$ axis yet, but it passes below two other terms in a vicinity of their crossing. Now the optimal

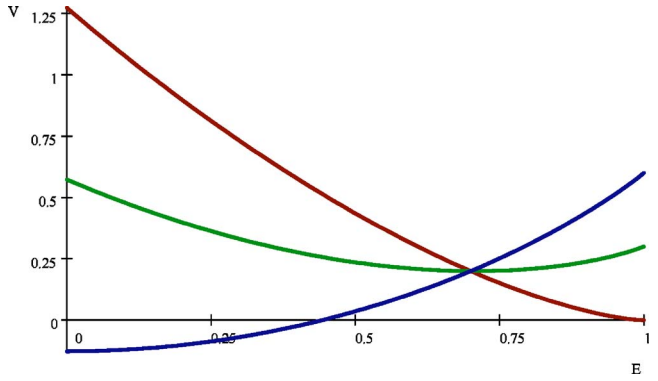

FIG. 6. (Color online) Tunneling branches $V_\nu-\nu U$ as a function of the energy E of the associated bound state. This figure corresponds to $U=1.4$ which is between the thresholds for tunneling of bipolarons and polarons.

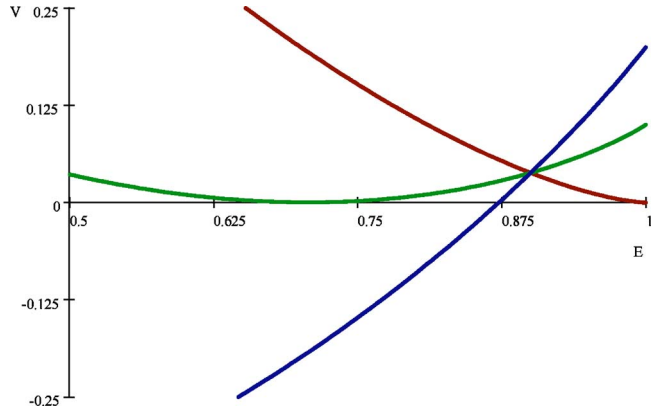

FIG. 7. (Color online) Tunneling branches $V_\nu - \nu U$ as a function of the energy E of the associated bound state (over a selected interval). This figure corresponds to $U=1.8$ which is just at the polaronic threshold, above the bipolaronic one.

bielectronic tunneling takes place via a sequence of two single electronic processes confined in time.

APPENDIX B: DERIVATION OF PREFACTOR

We need to perform the integration over $\Delta_j(x,t)$ around the extremal taking into account the zero modes related to translations of positions $X_j(t)$ of the instanton centers. The path integration over the gapless mode $X(t)$ is important, particularly for the matrix element: the overlap of wave functions evolves following $X_a(t)-X_b(t)$ while their localization follows the evolution of $E(t)$. We shall work within the zero-dimensional reduction of Eq. (12).

We expand the field $\Delta_j(x,t)$ in the vicinity of the instanton solution as

$$\Delta_j(x,t) = \Delta_0(x - X_j(t), E_j(t) + \delta[x - X_j(t), t]). \quad \text{(B1)}$$

Following Ref. 3, we rewrite Eq. (8) as

$$J \propto t_\perp^2 \prod_{j=a,b} \int d(x-y)d(\tau_1-\tau_2) \int D[E_j]D[X_j]J_{X_j}J_{E_j}\exp(-S)$$
$$\times \Psi_a^*[x - X_a(\tau_1), E(\tau_1)]\Psi_a[y - X_a(\tau_2), E(\tau_2)]$$
$$\times \Psi_b[x - X_b(\tau_1), -E(\tau_1)]\Psi_b^*[y - X_b(\tau_2), -E(\tau_2)], \quad \text{(B2)}$$

where $J_X = \propto \Pi_{n=1}^N \sqrt{M[E(t_n)]}$, $J_{E_j} \propto \Pi_{n=1}^N \sqrt{f[E_j(t_n)]}$ are the Jacobians of the transformation (12). ($N \to \infty$ is the number of points for the intermediate discretization of the time axis.) We integrate over the zero mode $X(t)$ and take into account fluctuations of the instanton shape due to variations of the parameter $E_0(t)$.

The action in Eq. (12) has the form

$$S[X,E] = \sum_{j=a,b} dt M[E_j(t)]\dot{X}_j^2/2 + f(E_j)\dot{E}_j^2/2 + V_U(E_j)$$

with $V_U(E)$ from Eq. (20). The integration over $DX_i(t)$ is carried out exactly after the transformation $M\dot{X}^2 = \dot{Z}^2$ using the known expression

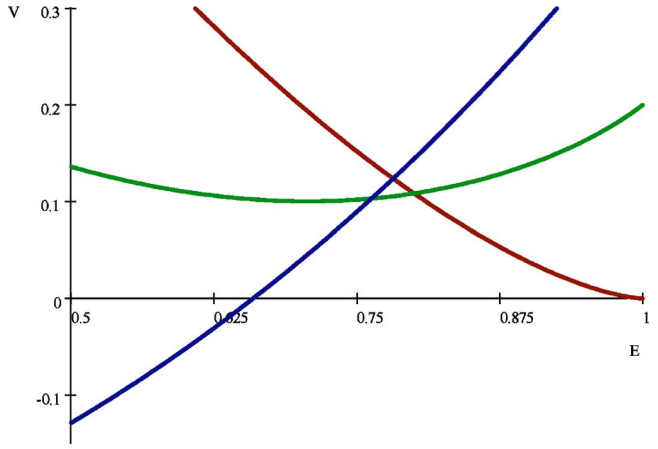

FIG. 8. (Color online) Tunneling branches $V_\nu - \nu U$ as a function of the energy E of the associated bound state. This figure corresponds to $U=1.6$ which is between the thresholds for tunneling of bipolarons and polarons. Contrarily Fig. 6, the Coulomb interaction is taken into account which lifts the crossing degeneracy.

$$\int D[x]\exp\left[-\int_{t_1}^{t_2} dt\left(\frac{\dot{x}^2}{2} + V(x)\right)\right] \sim \exp(-S_{\rm cl})\sqrt{\frac{d^2 S_{\rm cl}}{dx_1 dx_2}}, \quad \text{(B3)}$$

where $x_1 = x(t_1)$, $x_2 = x(t_2)$. Next, we perform in Eq. (B2) the remnant integrations over coordinates at the impact moments $X_1 = X_a(\tau_1)$, $X_2 = X_a(\tau_2)$, $Y_1 = X_b(\tau_1)$, $Y_2 = X_b(\tau_2)$:

$$J \propto t_\perp^2 \int dx d\tau_1 dX_1 dX_2 e^{-(X_1 - X_2)^2/l^2}\Psi_a^*[x - X_1, E(t_1)]$$
$$\times \Psi_a[y - X_2, E(t_2)]\frac{\sqrt{M_1}}{l_1} dY_1 dY_2 e^{-(Y_1 - Y_2)^2/l^2}$$
$$\times \Psi_b^*[x - Y_1, -E(t_1)]\Psi_b[y - Y_2, -E(t_2)]\frac{\sqrt{M_2}}{l_2}$$
$$\times \exp[-S_E(E)]. \quad \text{(B4)}$$

Here $M_i = M_i(\tau_{1,2})$, and the same for l_i, are functions of energies in these points which finally become $E_i = E_i(\tau_{1,2}) = U/2$. Using Fourier transforms, we rewrite the product of wave functions as

$$\int dp dq d\tilde{p} d\tilde{q} \Psi_{a,p}^* e^{-ip(x - X_1)}\Psi_{a,q} e^{iq(y - X_2)}$$
$$\times \Psi_{b,\tilde{p}} e^{i\tilde{p}(x - Y_1)}\Psi_{b,\tilde{q}} e^{-i\tilde{q}(y - Y_2)}.$$

Integration over $dxdy$ gives $\delta(p-\tilde{p})$, $\delta(q-\tilde{q})$ and integration over dX_2, dY_2 gives $L\delta(p-q)$. After integration over $d(X_1 - X_2)d(Y_1 - Y_2)$ we arrive at the result (15). The factor $\sqrt{dT/dU} = 1/\sqrt{d^2 S/dT^2}$ in Eq. (15) after integration over $D[E_i(t)]$ which was performed using Eq. (B3) again.[23]

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