Strings and Stripes in Ionic Solids

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Abstract

We demonstrate the existence of strings or electronic molecules in narrow band ionic insulators arising purely from the Fröhlich electron-phonon interaction alone. The system is in an inhomogeneous state in a wide range of physically interesting parameters, where the electronic molecules may coexist with the Fermi liquid. We show that conditions for string existence, the string length and the number of self-trapped particles depend on the electron(hole) conduction bandwidth and on the ratio of high frequency and static dielectric constants.

Key words: electronic clusters; Fermi liquid; polarons; bipolorons, strings; stripes

Recently we have introduced a notion of electronic molecules, generalizing the concept of polarons on many-body case[1], which may arise in solids due to electron-phonon interactions. We have shown that nearly all types of the electron phonon interaction lead to the creation of electronic molecules, which may be created either in a ground state or in a metastable state and have mostly a linear shape. Such structures are typically connected to *static or dynamic stripe phases* observed in oxides [2–6].

The electronic molecule is a many-particle generalization of a conventional polaron, which may be created both by a long- or short-range electron-phonon interaction[1]. Here we show that the Fröhlich interaction combined with direct Coulomb repulsion does lead to formation of strings coexisting with free electrons.

To describe these electronic molecules we consider a general Hamiltonian for spinless fermions interacting with phonons and with each other via long-range Coulomb forces and located on a three dimensional cubic lattice:

$$H = -t \sum_{<i,j>} a_i^\dagger a_j \quad + \sum_{q,i} \omega(q) n_i [u_i(q) b_q + h.c.] + \sum_q \omega(q) b_q^\dagger b_q \; + \sum_{i<j} V(i-j) n_i n_j, \qquad (1)$$

where t is the electron hopping-integral, the operator $a_i^\dagger(a_i)$ creates (destroys) a fermion at a lattice site i , n_i is the occupation number operator $a_i^+ a_i$ and the operator $b_q^\dagger(b_q)$ is the creation (destruction) operator of a phonon. The summations in eq.(1) extend over the lattice sites i and -as indicated by $< i, j >$ -over the associated nearest sites j. The matrix element of the electron-phonon interaction is equal to

$$u_n(q) = \frac{\gamma(q) \exp{(iqn)}}{\sqrt{2N}} \qquad (2)$$

The function $\gamma(q)$ and the phonon dispersion relation $\omega(q)$ are different for different types of electron-phonon interactions. For optical longitudinal phonons (Pekar-Frölich interaction) in the continuum limit the product $\gamma^2(q)\omega(q) = 4\pi e^2/(\epsilon^* q^2)$ with $1/\epsilon^* = 1/\epsilon_\infty - 1/\epsilon_0$. The function $V(i-j) = e^2/|i-j|\epsilon_\infty$ is a two-particle potential of the long-range Coulomb interaction[1].

We employ a Hartree-Fock many-body wave function, $\Psi(1, 2, ..., M)$, which is a Slater determinant

$$\Psi(1, 2, ..., M) = \frac{1}{\sqrt{M!}} \det \mid\mid \psi_{m_i}(k_j) \mid\mid \qquad (3)$$

consisting of normalised single particle wave functions:

$$\psi_{m_i}(k_j) = \begin{cases} \frac{1}{\sqrt{N}} \exp(ik_j m_i) & \text{if} \quad 1 \le m_i \le N \\ 0, & \text{otherwise} \end{cases} \qquad (4)$$

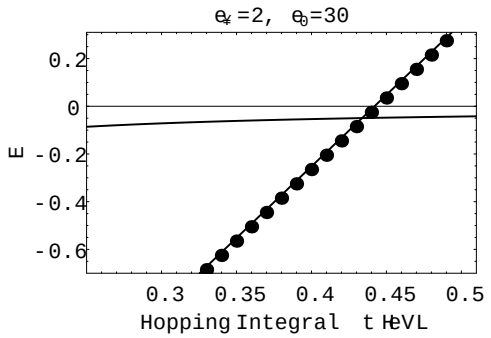

Fig. 1. The dependence of the total energy of the small and Pekar polarons (solid lines) and of strings (dots) on the hopping integral. The bottom of the conduction band is located at zero energy. With increasing hopping integral the number of particles in the string increases.

The value of total energy may be estimated with the use of the Pekar functional $J = T + V + V_c$ which includes the conventional kinetic and potential energy of fermions T and V, respectively, (see, Refs[1]) together with the Coulomb contribution, V_c, coming from the long-range Coulomb interaction between fermions located on the discrete lattice. The electronic molecule is determined by a minimization of the total energy J with respect to the length of the string N at the fixed value of the number of particles M trapped into the string.

Our investigation shows that if the ratio of dielectric constant is large enough (ie it is larger than some critical value) the optimal string energy per particle becomes smaller than the polaron energy provided that the bandwidth is smaller some other critical value,ie $t < t_c$. For an illustration we present the energy dependencies for strings and polarons on t in Fig.1 where the values of the dielectric constants are taken to be $\epsilon_0 = 30$ and $\epsilon_\infty = 2$.

Here, if the bandwidth or the hopping integral t is smaller than some critical value $t < t_c = .43eV$ the optimal string is the ground state (see, Fig.1). The value of t_c depends also on the ratio of the dielectric constants $\epsilon_0/\epsilon_\infty$, and increases when this ratio increases. For the chosen values of dielectric constants strings arise in ionic solids when the bare bandwidth is of the order of 1-2 eV or smaller. However with the next decrease of the bandwidth the string solutions collapse into a small polaron state to which the Pekar polaron state is transformed, too. There arises an abrupt transition from the string state to the small polaron state. In fact when the bandwidth changes the structure of the strings changes abruptly.

With decreasing bandwidth the length of the string and the number of particle trapped decreases, for example, first, a four particle string arises, then - a three-particle string(tri-polaron), then - a bipolaron and finally a last, final transition (like all other jumps) to a small polaron. Each string corresponds to a local minimum of the total energy and is separated from the other state by a barrier. Therefore, any of these transitions from one type of the string to the other type must go over the barrier. However the difference between the strings and polaron states is very small (all string dots are crossing the small polaron line, see, Fig.1). This means that for narrow bands all these types of strings and polarons will coexist with each other, ie they will create a "fog" of all types of electronic clusters. With increasing bandwidth this "fog" of electronic clusters will be embedded into a see of free fermions (an inhomogeneous Fermi liquid). It is important to note that for the wide bands the string corresponds to a metastable state, has a very large length and traps many particles. Here the continuum approximation for the number of particle trapped and for the length of the string gives reliable results[1]. On the other hand for narrow bands, when the string length decreases and inside the string associated with a ground state of the system there are only a few particles trapped the lattice discreteness must be properly taken into account.

In general the strings may correspond to either a ground state or a metastable state and arise typically when the bandwidth is not very large. With increasing bandwidth the ground state associated with these strings transforms into a metastable state while the string length and the string degeneracy increase. There may arise different physical situations, for example, phases of static and dynamic stripes, of superconducting and insulating states.

In summary, we have shown that strings may arise in ionic solids due to an interaction with Fröhlich phonons alone. Any other type of electron-phonon interaction taken into account strongly improves and increases the range of the physical parameters at which these strings arise in a ground state. We believe that such electronic molecules arising due to an interplay between Coulomb forces and electron-phonon interactions are a pertinent notion for oxides and possibly also for other novel materials.

References

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