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The influence of the interchain coupling on large acoustic polarons in coupled molecular chains: Three coplanar parallel molecular chains

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ABSTRACT

We study the properties of the single large adiabatic polaron in the substances composed of three parallel equally separated coplanar molecular chains. Particular attention has been devoted to the influence of the interchain coupling strength on polaron stability in order to elucidate the origin of the large polaron existence, which, contrary to the predictions of continuum adiabatic theories may persist in realistic conditions.

Our results indicate the existence of the effectively two-dimensional stationary polarons with comparably large longitudinal radius while the transverse one ranges from zero, in the absence of interchain coupling, to approximately twice of the interchain separation when coupling strength tends towards the infinity. These two-dimensional polarons are both energetically and dynamically stable. This is quite the opposite to the expectations based on the traditional adiabatic large polaron theories which, in the case of short – ranged electron–phonon interaction, predict that the stable large polaron may exist only in 1D systems. Stability of these 2D polarons increases with the increase of the interchain coupling strength so that they may be comparably more stable than the pure 1D polarons.

1. Introduction

The electronic properties of the low dimensional materials such as conjugated polymers [1–3], quasi-one-dimensional (Q1D) organic conductors [4–6] and biological macromolecules (DNA and α helical proteins) [7–14], have been the subject of the intensive investigations for many years. Due to the reduced dimensionality, electronic properties of these materials significantly differ from those in bulk media and cannot be described within the conventional band theory. In particular, as shown in a series of papers [15–22], even very weak electron–phonon interaction in pure 1D leads to polaron formation. Especially interesting situation may arise in the adiabatic and strong coupling limit when the large polaron formation takes place [15–22]. One-dimensional large polarons represent stable, mobile, quasi-particles capable to provide efficient long range charge and energy transfer in 1D systems, which motivated an extended discussion on the possible role of the polaronic mechanism in the transport processes in the actual Q1D substances [1–22].

These ideas are founded on the theoretical studies carried on within the idealized 1D models which cannot be directly applied to the actual Q1D materials which are highly anisotropic but truly three dimensional (3D) structures. Theoretical investigations [23,24] of large polarons carried out within the quasi-realistic models in which Q1D substances were modeled as a collection of the large number of parallel molecular chains, have indicated that

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the effectively 1D polaron confined to a single chain may exist within these structures under the very restricting conditions since even tiny interchain coupling may destabilize the large polarons. Despite these purely theoretical arguments, the existence of the 1D large polaron has been experimentally verified in some realistic Q1D media [25–27]. There are some indications that the additional anisotropy of the transverse and longitudinal electron bandwidths arising on account of the small-polaron effect [28,29] and the presence of the various defects such as chain endings and conjugation brakes [30,31] could produce the existence of the effectively 1D polaron, nevertheless, the origin of the polaron stabilization and confinement in these substances is not fully theoretically understood. For that reason, the possible role of the large polarons in the transfer processes in actual Q1D media in the presence of interchain coupling is still an open problem and attracts considerable attention of the number of researchers for years [32–41].

Gross of these studies were focused on a two-chain structures, such as DNA [7,8] and coupled conjugated polymer chains [2,3,37–41] due to their possible broad applications as the molecular wires in the design and fabrication of micro- and nano-sized electronic devices. It turns out that the large polarons in the two-chain structures exhibit specific features quite different from those in pure one, two or three-dimensional media. In particular, the polaron may be confined to a single chain or may be sited between them depending on the magnitude of the interchain transfer integral. In our recent article [42] we have generalized the results of the preceding studies on polarons in the two-chain structures establishing the criterion for the existence of the effectively 1D large acoustic polaron in these substances. The crucial role in that sense has the interchain coupling constant (γ) representing the ratio of the magnitude of interchain tunneling energy and the large polaron binding energy. Thus, in the weak interchain coupling regime, i.e. for the coupling constant bellow the critical value $\gamma < 1/2$, polaron is confined to a single chain. As the coupling strength increases, the continual transition towards the delocalization takes place – the polaron amplitudes on both chains gradually become equalized, in the same time, its binding energy vanishes. That is, the gradual de-confinement of the one-dimensional polaron takes place. This may be interpreted as polaron destabilization occurring at $\gamma > 1/2$. This value corresponds to approximately eight times lower threshold for the polaron existence then in the bulk media. More precisely, the anisotropy degree (the ratio of the intrachain over the interchain tunneling energy) required for large polaron existence in these substances is of the order of 12.5 [42] in contrast to 100 in the bulk materials [23].

Besides the two-chain form, realistic Q1D media may have a more complex structures embracing three or more chains. Therefore, further development of micro (nano) electronic devices and improvement of their performances, demands the investigations of the nature of charge and energy carriers and the elucidation of their transport properties in such more complex substances. This is a lot more challenging problem than in the two-chain substances since, even in the case of just three parallel chains, there are the variety of different possible particular structures, each of which may be modeled in a different way. Thus, for example, in the simplest case of three parallel identical mono-atomic or mono-molecular chains, planar (two-dimensional) and bulk, i.e. triangular actually three dimensional, arrangements of these chains are possible. Their electronic properties have to be investigated separately.

So far, the polarons or solitons in the three-chain structures have been studied mainly in the α-helical proteins [11–14] because of their fundamental role in the bioenergetics. In this article we study the properties of the single large adiabatic polaron in the substances composed of three parallel equally separated coplanar molecular chains. As for our best knowledge polarons and solitons in such structures were not studied so far. We particularly discuss the character of the large polaron and its stability in dependence of the interchain coupling strength in order to elucidate the origin of the large polaron existence, which, contrary to the predictions of the continuum adiabatic theories [23,24], may persist in realistic conditions. In addition, the present study could be of interest for the further understanding of the effects of the dimensionality on polaron. More precisely, the planar arrangement of the molecular chains represents the particular realization of the two-dimensional systems in which the polaron exhibits quite peculiar features [15–17].

Besides this general framework, our study may be relevant for some particular substances-β-sheet proteins [43], for example.

We adopt precisely the same theoretical model as in our preceding paper [42] and assume that the system parameters satisfy strong coupling and adiabatic limit where, in accordance with the general theory of the self-trapping phenomena [15–22,44,45], one may expect the large polaron formation in pure 1D media. Under these conditions, the theoretical investigations may be carried out by means of the time dependent version of the Pekar's semi-classical variational theory [15]. Its straightforward application in the present context results in a set of coupled nonlinear Schrödinger equations for the polaron wave functions on particular chains:

$$i\hbar\dot{\Psi}_j + Ja_0^2\frac{\partial^2\Psi_j}{\partial x^2} + G(v)|\Psi_j|^2\Psi_j - L(\Psi_{j+1} + \Psi_{j-1}) = 0,$$
$$G(v) = \frac{4E_B}{1-\frac{v^2}{c_0^2}}, \quad c_0 = a_0\omega_0, \tag{1}$$

where index j enumerates chains. Note that, due to the specific structure that we consider here, the polaron wave functions have to satisfy the following boundary conditions:

$$\Psi_j = 0 \quad \text{for} \quad j = 0 \quad \text{and} \quad j \geqslant 4. \tag{2}$$

Here v and c_0 denote polaron velocity and speed of sound, respectively, while a_0 stands for the lattice constant. Electronic subsystem is characterized by the intrachain J and interchain L electronic transfer integrals; lattice dynamics is determined by the maximal phonon frequency $\omega_0 = \sqrt{\frac{\kappa}{M}}$ in which M and κ stand for the molecular mass and the stiffness of the chain, respectively. Electron–phonon interaction is characterized by means of small polaron