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Vibrational modes in harmonic chains with diluted disorder

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Abstract

We study the nature of collective excitations in harmonic chains with diluted disorder. Using a transfer matrix method, we compute the localization length of eigenmodes within the band of allowed energies in order to investigate the new extended states which appear in this model. To follow the time evolution of an initially localized energy input, we calculate the second moment $M_2(t)$ of the energy spatial distribution. We found that for an impulse initial excitation, the super-diffusive energy spread is not affected by the presence of new resonant modes. However, the energy spread becomes faster for a displacement excitation.

Keywords: Vibrational modes; Localization; Anomalous diffusion

1. Introduction

Usually, disorder induces localization of collective excitations thus degrading transport properties. This effect is largely pronounced in low dimensions. In particular, the one-electron eigen-states in the 1D Anderson model with site-diagonal uncorrelated disorder are exponentially localized for any degree of disorder [1]. However, several 1D models with correlated disorder have been proposed which

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exhibit delocalized states [2–6]. Among these models, the diluted Anderson chain has attracted a renewed interest [7–11].

Hilke [7] introduced an Anderson model with diagonal disorder diluted by an underlying periodicity. The model consists of two interpenetrating sub-lattices, one composed of random potentials (Anderson lattice) and the other composed of non-random sites of constant potential. Due to the periodicity, special resonant energies appear. A similar model was used to study the electronic properties of semiconductor alloys [8]. The existence of an extended state at the band center was demonstrated, both analytic and numerically. The diluted Anderson model was extended to include a general diluting function which defines the on-site energies within each non-random segment [9]. Using a block decimation approach, it was demonstrated that this model displays a set of extended states, the number of which strongly depends on the length of the diluting segments and the symmetry of the diluting function. Recently, it was shown that the presence of new extended modes in the 1D diluted Anderson model promotes a sub-diffusive spread of an initially localized electron wave-packet [10]. The extension for a square lattice geometry has shown that this model can exhibit a true metal–insulator 2D transition with mobility edges delimiting a band of extended states [11].

The Anderson localization of collective excitation by a random potential is a quite general feature. It applies, for example, to the study of magnon localization in random ferromagnets [12]. Further, the collective vibrational motion of 1D disordered harmonic chains of N random masses can also be mapped onto an one-electron tight-binding model [13]. In such a case, most of the normal vibrational modes are localized. However, there are a few low-frequency modes not localized, whose number is of the order of $\sqrt{N}$ [13,14]. It was shown that correlations in the mass distribution produce a new set of non-scattered modes in this system [15]. Also, non-scattered modes have also been found in disordered harmonic chain with dimeric correlations in the spring constants [16]. By using analytical arguments, it was also demonstrated that the transport of energy in mass-disordered harmonic chains is strongly dependent on non-scattered vibrational modes as well as on the initial excitation [17]. For impulse initial excitations, uncorrelated random chains have a super-diffusive behavior for the second moment of the energy distribution [$M_2(t) \propto t^{1.5}$], while for initial displacement excitations a sub-diffusive spread takes place [$M_2(t) \propto t^{0.5}$]. The dependence of the second moment spread on the initial excitation was also obtained in Ref. [18]. Recently, several studies have been employed addressing the controversial question about the thermal conductivity behavior of mass chains in the thermodynamic limit [19–21].

In this work, we study the nature of collective excitations in harmonic chains with diluted disorder. The density of vibrational states is obtained, as well as accurate estimates for the Lyapunov exponent. These are used to characterize the new extended vibrational modes which appear in this model. In order to study the time evolution of an initially localized energy input, we calculate the second moment $M_2(t)$ of the energy spatial distribution. We show that these resonant modes are able to modify the dynamics of the energy spread.