# Elastic electron scattering and localization in a chain with isotopic disorder

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We study elastic electron scattering and localization by ubiquitous isotopic disorder in one-dimensional systems appearing due to an interaction with phonon modes localized at the isotope impurities. By using a tight-binding model with an intersite hopping matrix element dependent on the interatomic distance, we find a mass-dependent backscattering probability by single and pairs of isotopic impurities. For the pairs, in addition to the mass, the distance between the isotopes plays a critical role. Single impurities effectively attract electrons and can produce localized weakly bound electron states. In the presence of disorder, the electron free path at positive energies becomes finite and the corresponding Anderson localization at the spatial scale greatly exceeding the distance between the impurities becomes possible.

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## I. INTRODUCTION

Ubiquitous isotopic disorder leads to a finite zero-temperature resistivity even in metals where all other kinds of disorder do not exist. Since isotopic substitution does not produce an explicitly position-dependent random potential, the understanding and analysis of this residual resistivity is a highly nontrivial problem. This purely quantum effect based on the zero-point atomic motion was understood in Refs. [1,2]. The approaches of Refs. [1,2] are different. Reference [1] considered random kinetic energy of the lattice vibrations as the source of the electron scattering in terms of higher-order, beyond the first Born approximation, scattering theory. Later, it was shown in Ref. [2] that the Born approximation can be applied taking into account the randomization of the crystal lattice Debye-Waller factor by isotopic disorder. Both approaches result in a very small nonzero zero-temperature resistivity. Being the origin of unusual elastic and inelastic electron scattering [3], the isotopic disorder calls for studies of electron localization, usually considered as a result of a static randomly position-dependent potential, qualitatively different from the isotopic disorder producing a random field of dynamical finite frequency phonon modes. Here, we study these effects in a one-dimensional system [4] with isotopic disorder, where all the scattering processes can be presented in a clear explicit form.

Various aspects of the role of lattice vibrations for quantum transport have been studied for a long time (see, e.g., Refs. [5–9]). These approaches have been concentrated either on the zero-point motion of impurities [5–7] or on the effects of phonons [8,9] without taking into account the isotopic disorder. Here, we consider the aspect of this problem related to isotopic disorder specific for zero-point quantum motion in localized vibrational modes.

The problem of an electron interaction with isotopic disorder is directly related to the quantum impurity physics, where the electron interaction with an internal quantum structure of the impurity-related states strongly influences the electron kinetics. This interaction leads to inelastic scattering processes, as studied, e.g., in Ref. [10]. For isotopic defects the internal spectrum of the impurity is the localized vibrational mode. As we show below, this quantum effect can lead to elastic scattering eventually resulting in electron localization.

This paper is organized as follows. In Sec. II we briefly present already known results on localized phonon modes and electron-phonon coupling in the form required for the analysis of electron scattering by isotopic impurities. In Sec. III we formulate the scattering problem, identify corresponding virtual phonon process, and study elastic scattering by two configurations of isotopic impurities. Next, we show how the localization occurs and demonstrate its characteristic features. Conclusions and relations to other results will be given in Sec. IV.

## II. LOCALIZED MODES AND ELECTRON-PHONON COUPLING

### A. Eigenmodes with isotopic disorder

Vibrational eigenmodes in crystals of various dimensionalities with isotopic disorder have been studied for a long time and are well understood by now [11–16]. It is worth noting that several advanced numerical approaches [17,18] for these modes have been proposed recently to supplement mainly the analytical calculations of Refs. [11–16].

To provide a background for the following analysis of electron localization, we begin by presenting and analyzing some known results for an isotopically disordered chain with $N \gg 1$ atoms (see Fig. 1) described by the Lagrangian

$$\mathcal{L} = \tfrac{1}{2}(\dot{\mathbf{u}}^T \hat{M} \dot{\mathbf{u}} - \mathbf{u}^T \hat{K} \mathbf{u}), \tag{1}$$

 

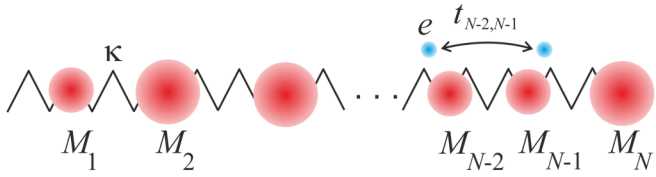


FIG. 1. Chain with isotopic disorder [cf. Eq. (2)]. Here, $\kappa$ is the elastic force constant, and $t_{n,n+1}$ is the electron bond-dependent hopping between two neighboring sites.

where $\mathbf{u}$ is the $N$ component vector of atomic displacements and the matrices given by:

$$\hat{M} = \begin{pmatrix} M_1 & 0 & 0 & \dots \\ 0 & M_2 & 0 & \dots \\ 0 & 0 & M_3 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix},$$
$$\hat{K} = \begin{pmatrix} 2\kappa & -\kappa & 0 & \dots \\ -\kappa & 2\kappa & -\kappa & \dots \\ 0 & -\kappa & 2\kappa & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \tag{2}$$

define the positions of isotopes with masses $M_n$ at the $n$th site, and elastic force constants, respectively. For calculations with Born–von Karman periodic boundary conditions one has $\hat{K}_{1,N} = \hat{K}_{N,1} = -\kappa$. The characteristic equation $\det[\hat{K} - \hat{M}\omega^2] = 0$ yields the corresponding $\{\omega_\alpha^2, \phi_n^\alpha\}$, where $\alpha = 1, \dots, N$ numerates the eigenmodes with eigenvectors $\phi_n^\alpha$ and statistical properties of the frequencies $\omega_\alpha^2$ distribution obtained in the pioneering paper of Dyson [11]. For the isotopically clean system we get $\omega^2(k) = \omega_B^2 \sin^2 ka_0/2$ ($\omega_B = 2\sqrt{\kappa/M}$ is the phonon frequency at the Brillouin zone boundary, and $a_0$ is the lattice constant of the chain) with $\phi_k(n) = e^{ika_n}/\sqrt{N}$ and $\sum_n \phi_k^*(n)\phi_{k'}(n) = \delta_{k,k'}$, where $a_n = na_0$ is the position of the $n$th site. The orthogonality and normalization condition reads as $(\mathbf{u}_\alpha^T \hat{M} \mathbf{u}_\beta) = \delta_{\alpha\beta}$.

The operator of the displacement vector in the second quantization form is given by

$$\hat{u}_n = \sum_\alpha \sqrt{\frac{\hbar}{2M\omega_\alpha}} (b_\alpha^\dagger + b_\alpha)\phi_n^\alpha, \tag{3}$$

where $b_\alpha$, $b_\alpha^\dagger$ are the Bose annihilation and creation operators, $M = \langle M_n \rangle$ is the average mass of atoms in a chain, and normalized $\phi_n^\alpha$ now includes dimensionless prefactor $\sqrt{M/M_n}$. To consider electron scattering by phonon modes one also needs the Fourier transformation

$$\hat{u}_q = (\boldsymbol{\phi}_q^* \cdot \hat{\mathbf{u}}) = \sum_\alpha \sqrt{\frac{\hbar}{2M\omega_\alpha}} (b_\alpha^\dagger + b_\alpha)\phi_q^\alpha, \tag{4}$$

where $\phi_q^\alpha$ is obtained from eigenvectors as

$$\phi_q^\alpha = (\boldsymbol{\phi}_q^* \cdot \boldsymbol{\phi}^\alpha) = \frac{1}{\sqrt{N}} \sum_n e^{-iqa_n} \phi_n^\alpha. \tag{5}$$

Here, we consider a realization with identical isotope impurities of masses $M_i$ being smaller than the mass $M$ of other atoms in the chain. For a single isolated isotope there exists one vibrational mode that splits off from the continuous spectra of phonons to form a bound state localized nearby [19]. For a small $|\Delta M|/M \ll 1$ (we restrict our consideration below to this realistic approximation) the frequency of this mode $\omega_{\rm loc} = \omega_B + \omega_B(\Delta M/M)^2/2$ lies slightly above $\omega_B$.

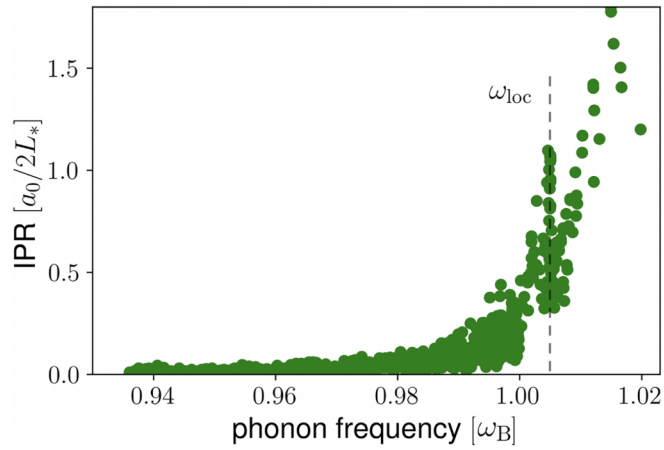


FIG. 2. IPR distribution of phonon modes for $\Delta M/M = -0.1$, $\nu_{\rm is} = 1/20a_0$, and the frequency of the localized mode $\omega_{\rm loc}/\omega_B \approx 1.005$.

The localized mode $\phi_n^{\rm loc}$ centered at $n_0$ is described by [19]

$$\phi_n^{\rm loc} = (-1)^{n-n_0} \sqrt{\frac{a_0}{L_*}} e^{-a_0|n-n_0|/L_*}, \quad \frac{a_0}{L_*} = 2\frac{|\Delta M|}{M}. \tag{6}$$

Here, $L_*$ is the mode localization length. The resulting Fourier structure of the isotope-related mode being localized and centered at the Brillouin zone boundaries $q = \pm q_B$, where $q_B = \pi/a_0$, can be presented, assuming $n_0 = 0$, in the Lorentzian form as

$$\phi_q^{\rm loc} = \frac{2}{\sqrt{Na_0}} \frac{1}{L_*^{3/2}} \times \left( \frac{1}{(q-q_B)^2 + L_*^{-2}} + \frac{1}{(q+q_B)^2 + L_*^{-2}} \right). \tag{7}$$

Since $\phi_n^{\rm loc} = \phi_{-n}^{\rm loc}$ is symmetric, the Fourier component $\phi_q^{\rm loc} = \phi_{-q}^{\rm loc}$ is real. The Fourier distribution of the localized mode has the width $L_*^{-1}$.

To characterize spatial localization of the modes we use the inverse participation ratio (IPR)

$$\mathcal{I}^\alpha = \sum_n \left(\phi_n^\alpha\right)^4, \tag{8}$$

where for delocalized modes $\mathcal{I}^\alpha = O(1/N)$. A single isotope impurity produces a localized mode with $\mathcal{I}^{\rm loc} \approx a_0/2L_*$. Other $N-1$ phonons are delocalized with the corresponding $\mathcal{I}^\alpha \ll a_0/L_*$ and do not have a smooth Fourier structure. In Fig. 2 we present the $\mathcal{I}^\alpha$ for a diluted disordered system where the mean distance between the light isotopes $1/\nu_{\rm is} = 4L_*$. The figure shows a clear distinction between localized and delocalized modes. It is interesting to mention that the mapping of phonon localization [20,21] on the Anderson localization [22] and the Green's function analysis [23] similar to Ref. [24] show that at a finite concentration of impurities low-frequency phonon modes are localized, albeit with a vanishing $\mathcal{I}^\alpha$ in the zero-energy limit (see Ref. [25] for review).

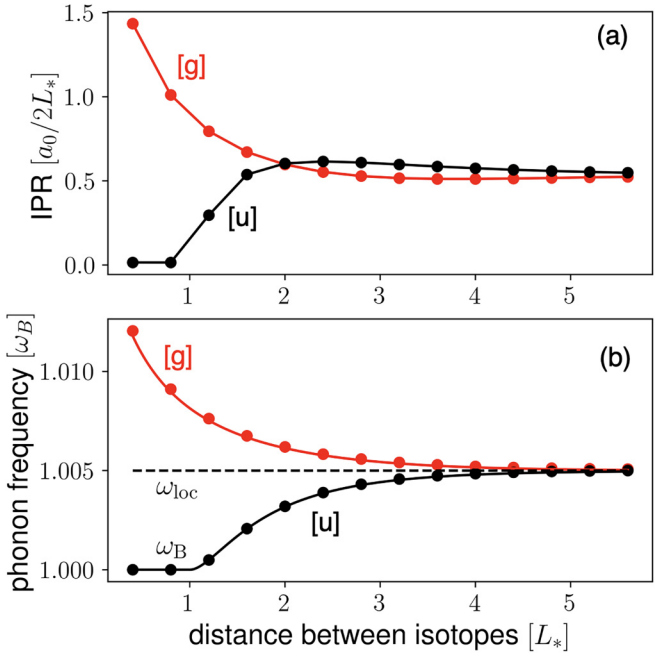


FIG. 3. (a) The IPR and (b) the frequency of two highest-frequency modes produced by a pair of isotopes as a function of the distance between them, $\Delta M/M = -0.1$.

Also, Fig. 2 indicates the presence of states with frequencies $\omega > \omega_{\rm loc}$ and larger $\mathcal{I}^{\alpha}$, suggesting smaller localization lengths. These states arise from isotopes located at the distances of the order of or less than $L_*$. Here, we consider two identical isotope impurities and for a qualitative analysis present the displacement as $u_n = (-1)^n u(x)$ and use a continual model [19] for the envelope function $u(x)$ with impurities presented as $\delta$ potentials at distance $a$,

$$s^2 u''(x) - a_0 \frac{\Delta M}{M} \omega_{\rm B}^2 [\delta(x - a/2) + \delta(x + a/2)] u(x) = 2\omega_{\rm B}(\omega - \omega_{\rm B}) u(x), \tag{9}$$

where $s = \omega_{\rm B} a_0/2$ is the speed of sound, resulting in the equation for $\omega$,

$$(2\xi - D)e^{\xi a} = \pm D, \tag{10}$$

with $\xi \equiv \sqrt{2\omega_{\rm B}(\omega - \omega_{\rm B})}/s$ and $D \equiv -a_0 \omega_{\rm B}^2 \Delta M/M s^2$.

Equation (10) implies that at a sufficiently small distance between the isotopes ($a < L_*$) only one (even) mode $u^{[\rm g]}(-x) = u^{[\rm g]}(x)$ remains localized with $\omega > \omega_{\rm B}$, while the other (odd) one, $u^{[\rm u]}(-x) = -u^{[\rm u]}(x)$, is pushed into the phonon continuum and becomes delocalized. These features are shown in Fig. 3, where we present the dependence of $\omega_{\rm loc}^{[\rm g,u]}$ and its $\mathcal{I}^{[\rm g,u]}$ on the distance $a$ between the isotopes. The corresponding Fourier components given by Eq. (5) are presented in Fig. 4.

### B. Electron-phonon interaction

We present the electron Hamiltonian in the tight-binding form

$$H = -\frac{1}{2} \sum_n t_{n,n+1} (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n), \tag{11}$$

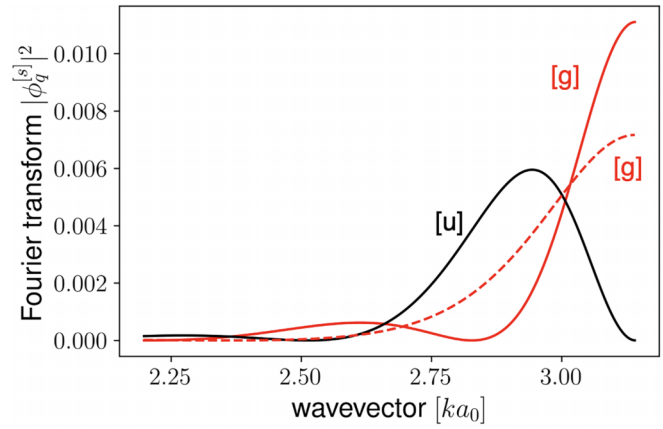


FIG. 4. Fourier $|\phi_q^{[s]}|^2$ for odd and even modes produced by pairs of isotope impurities, $|\Delta M/M| = 0.15$, $a = 10a_0$ (solid lines), and $a = 4a_0$ (dashed line). At $a = 4a_0$ the antisymmetric mode is delocalized and not shown here.

with the bond-dependent hopping (see Fig. 1) $t_{n,n+1} = t + \gamma'(u_{n+1} - u_n)$, with $c_n, c_n^\dagger$ being the electron annihilation and creation operators (irrelevant spin degrees of freedom are not included). In the electron momentum basis $c_k = N^{-1/2} \sum_n e^{-ika_n} c_n$ the phonon-independent term determines the one-dimensional electron dispersion $\varepsilon_k = -t \cos ka_0$. The noninteracting part of the Hamiltonian is given by

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_\alpha \hbar\omega_\alpha b_\alpha^\dagger b_\alpha. \tag{12}$$

The electron-phonon interaction part can be written as

$$H_{\rm e-p} = -\frac{i\gamma'}{\sqrt{N}} \sum_{k',k} f_{k',k} c_{k'}^\dagger c_k \hat{u}_q, \tag{13}$$

where $\hat{u}_q$ is given by Eq. (4) with $q = k' - k$, and the form factor $f_{k',k} = \sin k'a_0 - \sin ka_0$. It is also convenient to rewrite the interaction potential in the form that directly exploits $\phi_q^\alpha$,

$$H_{\rm e-p} = -i\gamma \sum_{k',k\alpha} f_{k',k} c_{k'}^\dagger c_k (b_\alpha^\dagger + b_\alpha) \sqrt{\frac{\omega_{\rm B}}{\omega_\alpha}} \phi_q^\alpha, \tag{14}$$

the electron-phonon interaction constant $\gamma = C(\hbar\omega_{\rm B}/\rho s^2 L)^{1/2}/2\sqrt{2}$, where $C = \gamma' a_0$ is the deformation potential of the chain, $\rho = M/a_0$ is the mass density, and $L = Na_0$ is the chain length.

To explicitly confirm the effect of isotopic impurities on the quantum fluctuations of the intersite distances and corresponding electron hopping, we introduce the correlation function [cf. Eq. (3)]

$$g_{n,l} = \langle (u_{n+l} - u_n)^2 \rangle = \sum_\alpha \frac{\hbar}{2M\omega_\alpha} \left(\phi_{n+l}^\alpha - \phi_n^\alpha\right)^2. \tag{15}$$

Figure 5 demonstrates the dependence of $g_{n,l}$ (in the units of $\hbar/2\omega_{\rm B}M$) on the lattice site $n$ in the vicinity of the isotope for different $l$. Though the localized phonon mode has a spatial size $L_*$, this scale is not reflected in the behavior of $g_{n,l}$. The latter is mainly determined by low-frequency phonons with small corrections appearing due to the mass defect $\Delta M$ at the isotope site. The increase in $g_{n,l}$ in the vicinity of the isotopic

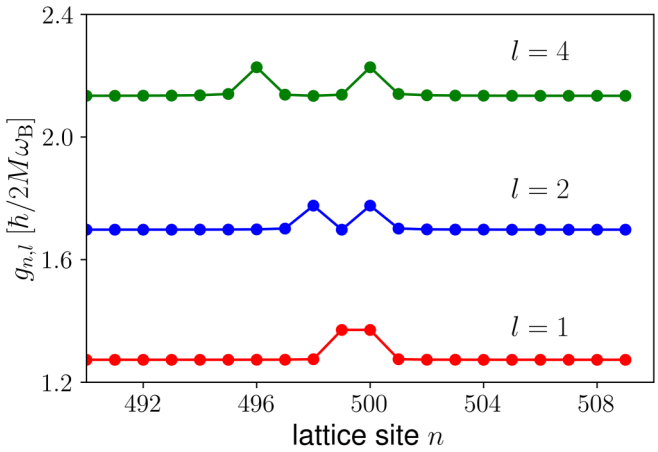


FIG. 5. Correlation function $g_{n,l}$ for different $l$ as marked near the plots. The isotopic defect is located at $n = 500$ and $|\Delta M|/M = 0.15$.

defect shows that the hopping integral fluctuates correspondingly and thus can influence the electron motion. However, as we will see below, the analysis of electron scattering cannot be reduced to using the only correlation function $g_{n,l}$.

## III. SCATTERING AND LOCALIZATION

### A. Elastic scattering by localized modes

Aiming at an analysis of localization we focus on the elastic electron scattering involving virtual phonon processes with the corresponding Feynman graph in Fig. 6. This process appears in the second order with respect to $\gamma$ and is due to the finite spread of phonon momentum in the presence of isotopes. The effective potential for an electron interacting with quantum vibrations in second order can be obtained following

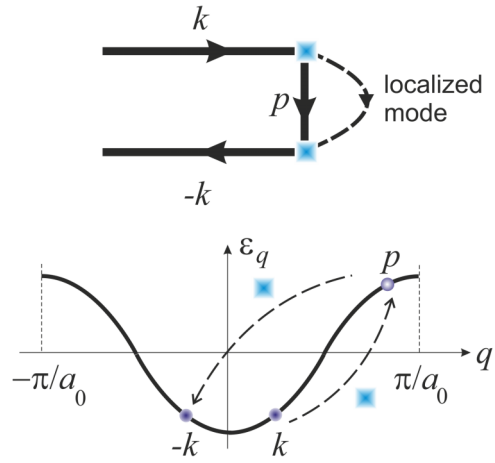


FIG. 6. A backscattering process. Solid squares correspond to matrix elements of electron-phonon coupling. Since the localized phonon mode has a spread in the momentum space, its virtual emission and absorption causes elastic electron backscattering with momentum change $-2k$. Notice that the main contribution to the real scattering process is due to the virtual transition to the Brillouin zone boundary with $|p| \approx \pi/a_0$.

Refs. [26,27] and is given by

$$\hat{V} = \tfrac{1}{2}[H_{e-p}, \hat{S}], \tag{16}$$

where [,] stands for the commutator and operator $\hat{S}$ is determined from $[\hat{S}, H_0] = H_{e-p}$. By taking the matrix elements of this commutator with respect to the eigenstates $(l, l')$ of $H_0$ (such as $|k1_\alpha\rangle \equiv c_k^\dagger b_\alpha^\dagger|0\rangle$, where $|0\rangle$ is the vacuum state), we obtain

$$S_{l,l'} = \frac{H_{e-p}^{l,l'}}{E_{l'} - E_l}. \tag{17}$$

To analyze the elastic scattering we first consider the matrix elements of $\hat{V}$ between $|k0\rangle$ and $|k'0\rangle$ phononless states. The explicit expression for this matrix element, $V_{k',k}$, is

$$V_{k',k} = \frac{1}{2}\sum_{p,\alpha}\langle k'0|H_{e-p}|p1_\alpha\rangle\langle p1_\alpha|H_{e-p}|k0\rangle \times\left(\frac{1}{\varepsilon_k - \varepsilon_p - \hbar\omega_\alpha} + \frac{1}{\varepsilon_{k'} - \varepsilon_p - \hbar\omega_\alpha}\right). \tag{18}$$

At small electron momenta the electron velocity $v_e = (d\varepsilon_k/dk)/\hbar = kta_0^2/\hbar$ and effective mass $m$ with $1/m = (d^2\varepsilon_k/dk^2)/\hbar^2 = ta_0^2/\hbar^2$. To avoid decoherence processes related to the emission of real phonons and suppressing the electron localization, we note that the no-emission condition $v_e < s$ restricts momentum to $k < k_{em}$, where $k_{em} = \hbar\omega_B/2ta_0$. Notice that the condition $t(k_{em}a_0)^2 \sim \hbar^2\omega_B^2/t \ll \hbar\omega_B$ prohibits the emission of real localized modes also. Using $H_{e-p}$ from Eq. (14) we keep in the sum of Eq. (18) only the modes corresponding to the localized states of Eq. (7) with frequency $\omega_\alpha = \omega_{loc}$. For a low concentration of single isotopes with a small mass defect, the Fourier components of other, delocalized, phonon modes with the frequencies lying within the phonon band spectrum, do not acquire a width sufficient to contribute to the sum of Eq. (18). Thus, we arrive at the matrix element of the electron scattering by a single isotope impurity:

$$V_{k',k}^{[1]} = -\frac{\gamma^2}{t}\Gamma_{k',k}^{[1]},$$
$$\Gamma_{k',k}^{[1]} = \frac{1}{2}\sum_p f_{k',p}f_{p,k}\phi_{k'-p}^\alpha\phi_{p-k}^\alpha\left(\frac{1}{\Delta(p,k)} + \frac{1}{\Delta(p,k')}\right),$$
$$\Delta(p,q) = 2k_{em}a_0 - \cos pa_0 + \cos qa_0. \tag{19}$$

The plot of $\log_{10}\Gamma_{k',k}$ corresponding to $V_{k',k}^{[1]}$ presented in Fig. 7 demonstrates that the scattering matrix element is relatively large only in the $q \lesssim L_*^{-1}$ range. The resulting calculated weakness of backscattering is due to two factors: a small allowed momentum transfer with $q = 2k \lesssim L_*^{-1}$, arising from the $\phi_p^{loc}\phi_{p+q}^{loc}$ [see Eq. (7)], and small $f_{k,p}$ at small $k$ and $p \approx q_B$. By using the condition $k_{em}a_0 \ll 1$ and expression for $\phi_q^{loc}$ in Eq. (7), we obtain

$$|V_{-k,k}^{[1]}|^2 = \left(\frac{\gamma^2 a_0^2}{2tL_*^4}\right)^2\frac{1}{(k^2 + L_*^{-2})^2}. \tag{20}$$

In the $kL_* \ll 1$ limit $|V_{-k,k}^{[1]}|^2$ behaves as $(\Delta M/M)^4$ and decreases as $(\Delta M/M)^8/k^4$ at $k \gg 1/L_*$. Equations (19) and (20)

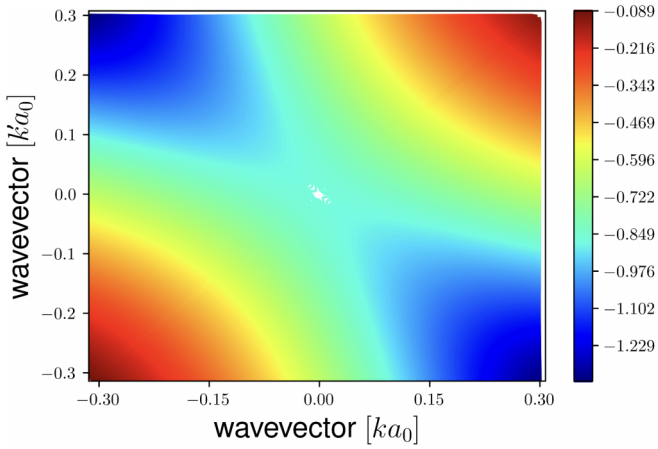


FIG. 7. Logarithm of matrix element $\log_{10}\Gamma_{k',k}$ for $\Delta M/M = -0.15$.

present the key result of this paper: Quantum isotopic impurities characterized by localized finite-frequency phonon modes can produce elastic electron backscattering. The corresponding numerically calculated $|\Gamma^{[1]}_{-k,k}|^2$ is presented in Fig. 8.

Having demonstrated possible elastic scattering by a single isotopic impurity, we can study how this general approach can be applied for two closely related impurities, where the interference of scatterings by odd and even vibrational modes plays a qualitative role, and see the characteristic features of this scattering. The matrix element of backscattering by two-isotope states, corresponding to Figs. 3 and 4, has the form

$$V^{[2]}_{-k,k} = -\frac{\gamma^2}{t}\Gamma^{[2]}_{-k,k|a},$$
$$\Gamma^{[2]}_{-k,k|a} = \sum_{p,[s]} \frac{1}{\Delta(p,k)} f_{-k,p} f_{p,k} \phi^{[s]}_{-k-p} \phi^{[s]}_{p-k}, \qquad (21)$$

and shows interference of the scattering processes. The corresponding probabilities are presented in Fig. 9. It is worth mentioning an increase in the scattering probability when two

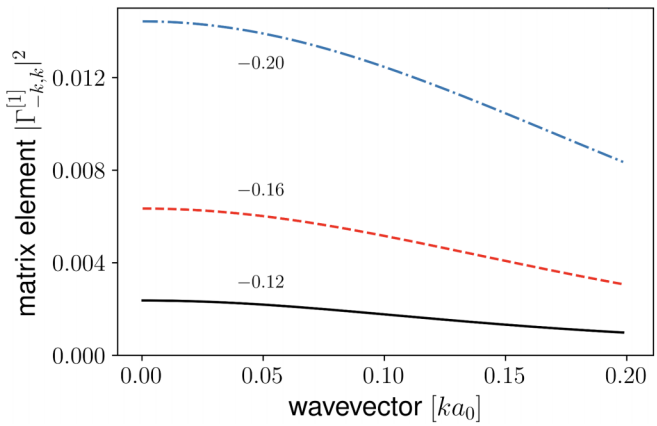


FIG. 8. $|\Gamma^{[1]}_{-k,k}|^2$ for $\Delta M/M$ shown near the curves. Fit according to Eq. (20) is not shown since it almost coincides with the numerical curves. The parameter $k_{\rm em}a_0 = 0.2$.

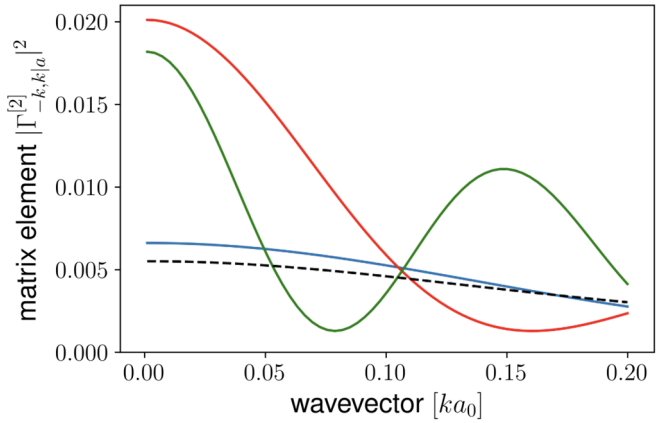


FIG. 9. Backscattering probability by two-isotope phonon states. Here, $\Delta M/M = -0.15$, $k_{\rm em}a_0 = 0.2$. The distance between isotopes: $a = 2a_0$ (blue), $a = 10a_0$ (red), $a = 20a_0$ (green). The dashed line corresponds to a single isotope.

isotopes are located at $a \lesssim 4L_*$, indicating a stronger scattering.

### B. Low density of impurities: Possible single-impurity localization and free path

As we demonstrated in the previous section, at small isotopic defects concentrations, a disordered chain can be presented as a randomly spaced ensemble of elastic scatterers, corresponding to scattering by a single and pairs of isotopic impurities. We assume a sufficiently small concentration of isotope impurities $\nu_{\rm is} \ll |\Delta M|/Ma_0$ such that they behave as independent single scatterers located at uncorrelated points $x_i$. The resulting small concentration of isotope pairs of the order of $\nu_{\rm is}^2 L_* \ll \nu_{\rm is}$ does not modify the localization-related results.

We begin with the quantum mechanical analysis of the electron free path in this system, where the finite free path indicates localization behavior and assuming that the main effect is due to single scatterers. In this analysis we use the one-dimensional free-space electron Green's function in the form

$$G_E^{(\pm)}(x,x') = \pm\frac{im}{k\hbar^2}\exp(\pm ik|x-x'|), \qquad (22)$$

where $E = \hbar^2k^2/2m$. Using the Green's function from Eq. (22) we obtain in the first Born approximation for scattering by a single isotope impurity located at a point $x_i$,

$$\Psi = e^{ik(x-x_i)} + r(k)e^{-ik(x-x_i)},$$
$$r(k) = -\frac{im}{\hbar^2 k}\widetilde{V}^{[1]}_{-k,k}, \qquad (23)$$

where $x < x_i$, $|x-x_i| \gg L_*$, $\widetilde{V}^{[1]}_{-k,k} = LV^{[1]}_{-k,k}$, and one expects $|r(k)| \ll 1$ as the approximation validity condition. The sign of $\widetilde{V}^{[1]}_{-k,k}$ is negative corresponding to an attractive potential of the width $L_*$, depth of the order of $t\times(\hbar\omega_{\rm B}/Ms^2)\times(a_0/L_*)^3$, and the binding energy $\epsilon_{\rm loc}$ of the order of $t(\hbar\omega_{\rm B}/Ms^2)^2(a_0/L_*)^4$. Here, we used relations $Ms^2 = \kappa a_0^2$ to scale the energy in dimensionless units and $t \sim C = \gamma' a_0$ by assuming that the intersite hopping integral

is sufficiently modified at the modulation in the interatomic distance of the order of $a_0$ [cf. Eq. (14)].

In the positive energy domain, the mean free path due to backscattering by isotopes can be estimated as $\ell(k) = \nu_{\rm is}^{-1}|r(k)|^{-2} \gg \nu_{\rm is}^{-1}$, corresponding to the Anderson localization at the spatial scale of the order of $\ell(k)$. Indeed, $|r(k)|$ is very small almost in the entire interval of $k < k_{\rm em}$ at the energies $\varepsilon_k + t > 10^{-2}(\Gamma^{[1]}_{-k,k})^2(\hbar^2/Ma_0^2)(t/Ms^2)$. At smaller energies, $|r(k)|$ approaches 1 and more detailed scattering approaches [24,28] have to be applied. To characterize the scattering, one can introduce dimensionless parameters $k_{\rm em}L_* \sim (\hbar\omega_{\rm B}/t)(M/|\Delta M|)$ and $\omega_{\rm B}\tau \sim M/|\Delta M|$, where, due to the condition $v_e < s$, the parameter $\tau = L_*/s$ represents the upper limit of the scattering time. Although $k_{\rm em}L_*$ can be either smaller or greater than 1, the product $\omega_{\rm B}\tau$ is always much larger than 1. This implies that scattering by isotopic impurities is an adiabatic process with low probability due to averaging of the intersite hopping during the scattering leading to the adiabatic limit for the binding energy $\epsilon_{\rm loc} \ll \hbar\omega_{\rm B}$.

### C. Electron localization

Here, we concentrate on electron localization by using the result of previous sections on mapping of isotopic impurities in chains on weak scatterers of electrons. As it was shown in Ref. [29], one-dimensional arrays of random scatterers lead to the localization of light waves with the same approach valid for the localization of electron waves.

Several approaches including the Lyapunov exponent analysis (e.g., Ref. [30]) and random matrix theory (e.g., Ref. [31]) can be used for studies of wave localization in random potentials. We will use a direct numerical calculation proving electron localization by producing a random potential corresponding to isotopic scatterers and calculating electron eigenstates in this potential. To study the localization, we consider a normalized electron wave function on an $N \gg 1$ site one-dimensional lattice, where $\psi_i(n)$ $(n = 1, \ldots, N)$ enumerates the lattice sites and $i$ enumerates the electron states with the energies $\varepsilon_i$. The probability density distribution for the state $i$ is characterized by the corresponding inverse participation ratio,

$$\xi_i = \sum_n |\psi_i(n)|^4. \tag{24}$$

The results for $\log_{10}\xi_i$ presented in Fig. 10 demonstrate the formation of two groups of localized states. The first group corresponds to the impurity band formed below the bottom of the conduction band with $\varepsilon_i < -2t$ [16]. The second group corresponds to the Anderson localization of the states inside the conduction band with $\varepsilon_i > -2t$. We notice that, as expected, the states become delocalized at the energies corresponding to $k > 1/L_*$, where the backscattering probability is strongly suppressed, according to Eqs. (23) and (20), where $V^{[1]}_{-k,k}$ behaves as $1/(k^2 + L_*^{-2})$, rapidly decreasing with the electron energy. Further, in Fig. 11 we present several typical wave functions $\psi_i(n)$ demonstrating that the Anderson localization occurs on a spatial scale much larger than the distance between the isotopic impurities.

Finally, we emphasize that our approach is qualitatively different from that proposed in Refs. [32–35]. The analysis

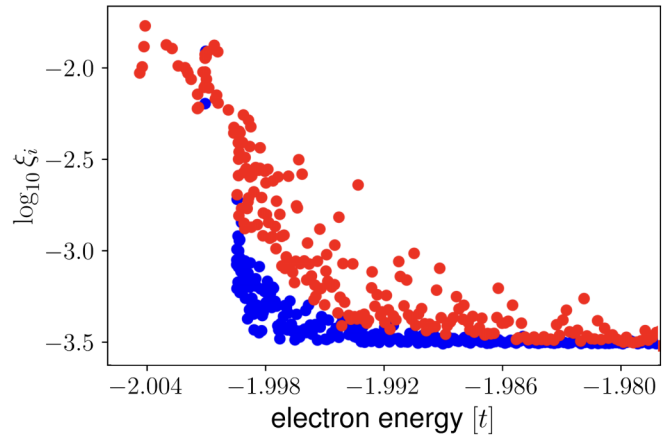


FIG. 10. The $\log_{10}\xi_i$ of the inverse participation ratio for two low-density distributions of isotopic impurities. The concentration of impurities $\nu_{\rm is} = 0.002$ (blue circles) and $\nu_{\rm is} = 0.009$ (red circles). The impurity width $L_* = 5a_0$ corresponding to $\Delta M/M = -0.1$ and the effective potential amplitude is $\tilde{V} = -0.01$. The hopping integral $t = 1$.

in these papers is based on the fact that the electron self-energy due to electron-phonon coupling, producing band-gap renormalization, is proportional to the dependence on the atomic masses' mean inverse phonon frequency [27]. Thus, clusters of isotopic impurities with sufficiently large size and concentration, renormalizing locally the electron band gap, can produce effective "potentials" able to localize sufficiently heavy carriers. Our approach is unrelated to the band-gap renormalization and electron localization occurs due to elastic scattering by randomly distributed localized phonon modes.

## IV. CONCLUSIONS AND OUTLOOK

We studied the localization of electrons due to a weak isotopic disorder producing randomly spatially distributed localized phonon modes in one-dimensional systems described

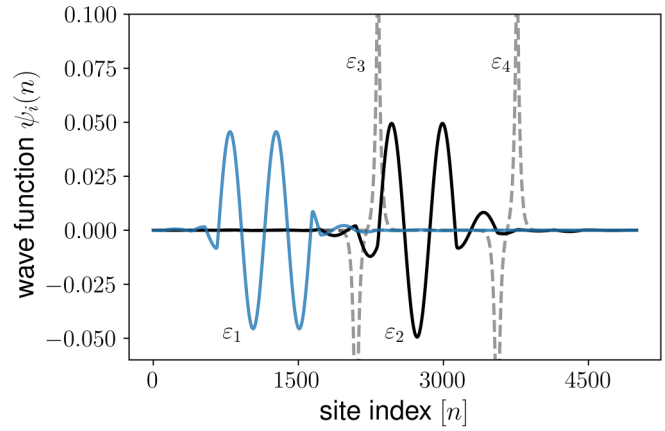


FIG. 11. Electron wave functions in different states with energies presented near the plots. Dashed lines: states in the impurity band with $\varepsilon_4 + 2t = -5 \times 10^{-6}t$ and $\varepsilon_3 + 2t = -1.4 \times 10^{-3}t$. Solid lines: states in the conduction band described by the Anderson localization with $\varepsilon_2 + 2t = 2.4 \times 10^{-4}t$ and $\varepsilon_3 + 2t = 3.4 \times 10^{-4}t$.

by a tight-binding model. Elastic electron scattering involving nonlocal processes of virtual emission and absorption of these modes is presented in the form of scattering by a weak potential with a strongly energy-dependent reflection probability. This randomness, related to the virtual phonon emission and absorption processes, leads to the Anderson localization with the localization length dependent on the electron energy. Investigations of more complex realizations including the formation of random weak-coupling polarons due to a strong isotopic disorder and possible effects of lattice nonlinearity (see, e.g., Ref. [36]) are of interest and will be a topic of future research.

To conclude the discussion of the effect of isotopic mass on the electron position in systems with different isotopes that emphasizes its general character, we mention that this effect is related to the puzzling dipole moment of the HD molecule [37], where different amplitudes of zero-point vibrations of hydrogen and deuterium ions lead to a shift of the electron probability density between these atoms resulting in the formation of a small dipole moment [37,38].

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