Density of Quasilocalized States Along the Resonance Curves in Continuum

A. M. Kosevich[1], D. V. Matsokin[2,*], and S. E. Savotchenko[3]

[1] *Verkin Physicotechnical Institute of Low Temperatures, National Academy of Sciences of Ukraine, Kharkov, 61103 Ukraine*

[2] *Kharkov National University, Kharkov, 61077 Ukraine*

** e-mail: matsokin@univer.kharkov.ua*

[3] *Belgorod State University, Belgorod, 308007 Russia*

Densities of quasilocalized states are calculated and analyzed for a one-dimensional system with a point defect and an FCC crystal with a planar defect. The density of states displays a pronounced peak that is positioned near the energy (frequency) of resonant transmission of a particle (wave) through the defect but slightly shifted from this energy. The peak nears the resonance frequency and sharpens, tending to a δ function, as the continuum edge is approached.

In recent years, considerable interest has been expressed in the phenomena associated with the interaction of free propagating waves or particles with single-type states localized near the defects. In this respect, the specific features of a multichannel resonance scattering prove to be the subject of discussion [1– 3]. These features are closely related to the properties of quasilocalized states in a continuum [4]. The purpose of this work is to analyze the interconnection between the scattering amplitudes and the spectral density of states in the system of interest. Two examples are taken for the analysis: the interaction of two particles with different dispersion laws in a one-dimensional quantum system and the resonance phonon scattering in an FCC crystal containing a planar defect.

In Section 1, the amplitudes for particle scattering from a point defect are analyzed for a one-dimensional system with two types of elementary excitations that differ in the parameters of quadratic dispersion laws. At certain values of these parameters, the so-called Fano resonances appear in this system (an analogous situation was observed for the electron scattering from an impurity in a 2D quantum channel [2]). The density of quasilocalized states is calculated. It is shown that its maximum is fixed to the resonant transmission energy but slightly shifted from it.

In Section 2, the density of quasilocalized states is analyzed using the model of a planar discrete defect in an FCC crystal with the central nearest-neighbor interactions. The spectra of resonance modes and the in-gap localized states were calculated for this model in [5]. The density of quasilocalized states has a pronounced peak that is slightly shifted from the frequency of resonant transmission of elastic wave through the planar defect. It is shown that, on approaching the continuum edge, the peak comes closer to the resonant frequency and sharpens, tending to a δ function. Beyond the continuum, the resonance curve is continued as a dispersion curve for the in-gap state localized near the defect.

1. Density of states in a 1D system with two dispersion branches. A 1D quantum system with two groups of quasiparticles having quadratic dispersion laws are considered:

$$E = E_1 + \frac{k^2}{2m_1}, \quad E = E_2 + \frac{k^2}{2m_2}, \quad E_1 < E_2, \tag{1}$$

where Planck's constant $\hbar$ is taken to be unity. If a passive point defect is located at $x = 0$ in this system, the interaction with this defect, according to [3], can be written in the form of the following local potential:

$$\begin{aligned} H_{\text{int}}(x, x') &= U_0\{\alpha_1|\psi_1(0)|^2 + \alpha_2|\psi_2(0)|^2 \\ &+ \beta[\psi_1^*(0)\psi_2(0) + \psi_2^*(0)\psi_1(0)]\}\delta(x)\delta(x'), \end{aligned} \tag{2}$$

where $\psi_1(x)$ and $\psi_2(x)$ are the wave functions of the particles of the first and second type, respectively.

Let the particle of the first type with energy E ($E_1 < E < E_2$) be incident on the defect from the left. The second particle with this energy can only be in the localized state with wave function

$$\psi_2 = Be^{-\kappa|x|}, \quad \kappa = \sqrt{2m_2(E_2 - E)}. \qquad (3)$$

It was shown in [3] that the scattered particle can resonantly transmit through the defect at a certain ratio between its energy and interaction parameters. The interaction of a freely propagating particle of the first type with the localized state of the second type is the physical reason for the appearance of a resonance in the transmission through the passive defect. The total transmission occurs at $\alpha_1\kappa = m_2U_0(\beta^2 - \alpha_1\alpha_2)$.

We now intend to show that the energy corresponding to the total defect transparency correlates with the density of stationary quasilocalized states. The point is that in the system of interest quasilocalized states occur in the energy interval $E_1 < E < E_2$ for which the wave function ψ_1 has the form of a standing wave

$$\psi_1(z) = \begin{cases} A\cos(kx - \varphi), & x < 0 \\ A\cos(kx + \varphi), & x > 0, \end{cases} \qquad (4)$$

while ψ_2 is localized near the defect, according to Eq. (3).

The spectrum of quasilocalized states is continuous and characterized by a single parameter—phase φ. Making use of the boundary conditions following from the presence of the potential H_{int}, one can easily obtain the relation for the phase φ

$$\tan\varphi = \Delta_r(E)/\Delta_t(E), \qquad (5)$$

where

$$\Delta_r(E) = m_1U_0\{m_2U_0(\beta^2 - \alpha_1\alpha_2) - \alpha_1\kappa\},$$

$$\Delta_t(E) = k(\kappa + \alpha_2m_2U_0), \quad k = \sqrt{2m_1(E - E_1)}.$$

The addition to the bulk density of states is given by the formula

$$\delta g(E) = \frac{1}{\pi}\frac{d\varphi(E)}{dE} = \frac{1}{\pi}\frac{\Delta'_r(E)\Delta_t(E) - \Delta_r(E)\Delta'_t(E)}{\Delta_r^2(E) + \Delta_t^2(E)}. \qquad (6)$$

Assume that the total transmission occurs in the system $[\Delta_r(E_t) = 0]$. Assume also that the functions $\Delta_r(E)$ and $\Delta_t(E)$ vary smoothly near E_t; i.e., the point $E = E_t$ is positioned far from any spectral singularities (edges of spectral branches, etc.). Then, expanding in powers of $\delta E = E - E_t$ in Eq. (6), one obtains in the leading approximation

$$\delta g(E) = \frac{1}{\pi}\frac{\Gamma}{(\delta E + \Delta_t\Delta'_t/(\Delta_t'^2 + \Delta_r'^2))^2 + \Gamma^2}, \qquad (7)$$

where $\Gamma = \Delta'_r\Delta_t/(\Delta_r'^2 + \Delta_t'^2)$, $\Delta_{t,r} \equiv \Delta_{t,r}(E = E_t)$, and $\Delta'_{t,r} \equiv \Delta'_{t,r}(E = E_t)$. This expansion is valid if Δ'_t does not tend to zero; i.e., it is valid except for the cases

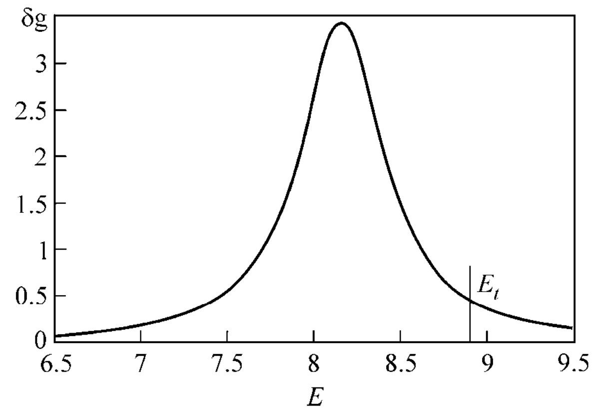

Fig. 1. The addition to the density of states as a function of energy; $U_0 = -0.7$, $m_1 = 1$, $m_2 = 2$, $\alpha_1 = 2$, $\alpha_2 = 2$, $\beta = 1$, $E_1 = 0$, and $E_2 = 10$. E_t is the total transmission energy.

when

$$E^* - E_t \ll E_t - E_1, E_2 - E_t,$$

where

$$E^* = \frac{1}{8}(8E_1 + 8E_2 - \alpha_2^2U_0^2m_2 + [32E_1^2 + 32E_2^2 + 192E_1E_2 + \alpha_2^4U_0^4m_2^2 - 16E_1\alpha_2^2U_0^2m_2)]^{1/2}.$$

One can see that the density of states near the point $E = E_t$ has the form of a Lorentzian peak with width Γ and center shifted from the E_t point by $\Delta_t\Delta'_t/(\Delta_t'^2 + \Delta_r'^2)$ (Fig. 1).

2. Density of states in an FCC crystal with planar defect. Let us consider the dynamics of an FCC crystal with a planar defect coinciding with the (001) plane. The coordinate axes are directed along the cube edges, and the z axis is perpendicular to the defect plane. Only the interactions between the nearest neighbors are considered. Following [5], we assume that the defect is characterized by a change in the force constant between the atoms belonging to the layers $z = 0$ and $z = -1$ (the edge of the unit-cell cube is taken to be 2). The ratio of force constant in the defect layer to the force constant in the pure crystal is denoted by ε.

It was shown in [5] that eigenmodes (including quasilocalized) in this crystal may be of two types, symmetric and antisymmetric. We are interested in the symmetric modes, for which

$$u_x^+(n_z - 1) = -u_x^-(-n_z), \quad u_z^+(n_z - 1) = u_z^-(-n_z),$$

where u_i^+ is the displacement in the upper half-space ($n_z \geq 0$), u_i^- is the displacement in the lower half-space ($n_z < 0$), and n_z numbers the atomic layers along the z axis.

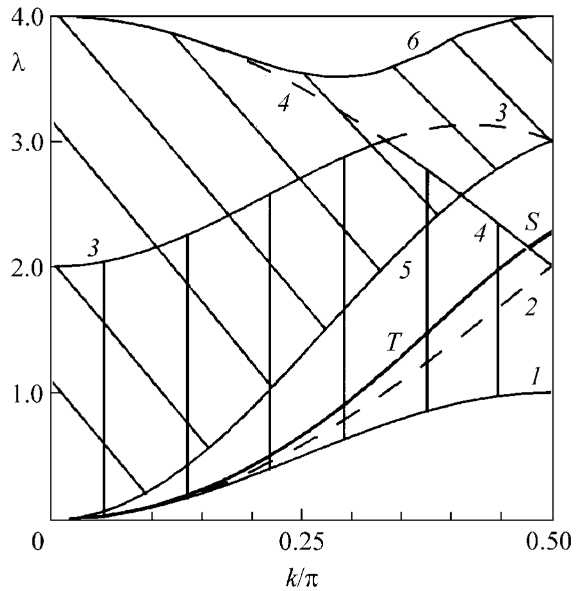

Fig. 2. Dispersion curves for the total transmission frequency T and symmetric vibration S for $\varepsilon = 3$. The vertical dashes correspond to the pseudotransverse branch, and the inclined dashes correspond to the pseudolongitudinal branch. Curve *2*: $\lambda = 2(1 - \cos k)$, $q = 0$; curve *3*: $\lambda = 2 - \cos 2k - \cos k$, $q = \pi$; curve *4*: $\lambda = 2(1 + \cos k)$, $q = \pi$; curve *5*: $\lambda = 2 - \cos 2k + \cos k$, $q = 0$; curves *1* and *6* are the lower and upper spectrum edges, respectively.

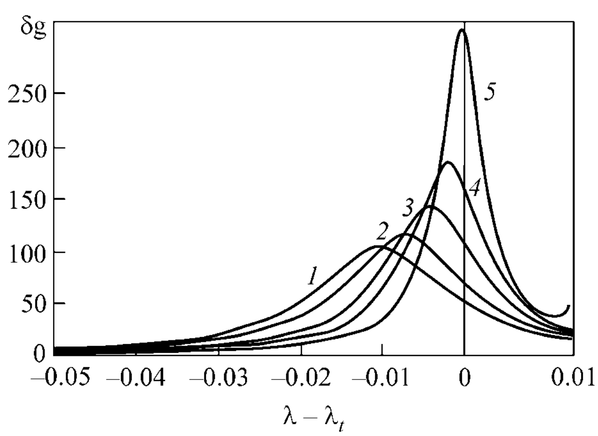

Fig. 3. Density of states as a function of $\lambda - \lambda_t$ for different k along curve T; λ_t corresponds to the total transmission frequency. Curves: (*1*) $k = 84\frac{\pi}{180}$; (*2*) $k = 85\frac{\pi}{180}$; (*3*) $k = 86\frac{\pi}{180}$; (*4*) $k = 86.5\frac{\pi}{180}$; and (*5*) $k = 86.9\frac{\pi}{180}$. $\varepsilon = 3$.

The resonant transmission and reflection take place for the phonons whose frequencies lie within one of the bulk crystal vibration branches but outside of the other branch. In these spectral regions, the quasilocalized eigenmodes may exist; i.e., two-partial modes, one component of which is localized near the defect while the other freely propagates in the crystal.

Let us consider a wave propagating in the [110] direction. This wave has two independent components: lower frequency (pseudotransverse) component, whose spectrum is vertically dashed in Fig. 2, and higher frequency (pseudolongitudinal) component, whose spectrum is shown by the inclined dashes in Fig. 2. In this case, there are three spectral regions where the quasilocalized states may exist (Fig. 2): the first one is bounded by curves *2*, *5*, and *4*; the second one is bounded by the solid section of curve *3* and dashed section of curve *4*; and the third region is bounded by curve *5*, solid section of curve *4*, and dashed section of curve *3*. Curve T in the low-frequency region of quasilocalized states corresponds to the total transmission conditions for the pseudotransverse wave through the defect. In the right part of Fig. 2, this curve meets the edge of the gap between the pseudotransverse and pseudolongitudinal frequency branches. Then, it is continued as curve S for the in-gap wave localized near the defect.

Let us consider the low-frequency region of quasilocalized modes. The wave displacement vector has the following form at $z \geq 0$:

$$\begin{aligned} \overset{+}{u}_x(x, z) &= (u_t \cos(qz + \varphi) + u_l e^{-\kappa z}) e^{ik(x+y)}, \\ \overset{+}{u}_z(x, z) &= (i u_t \Gamma_t \sin(qz + \varphi) + u_l \Gamma_l e^{-\kappa z}) e^{ik(x+y)}, \end{aligned} \quad (8)$$

where

$$\Gamma_t = -\frac{2 - \cos 2k - \cos k \cos q - \lambda}{\sin k \sin q},$$

$$\Gamma_l = i\frac{2 - \cos 2k - \cos k \cosh \kappa - \lambda}{\sin k \sinh \kappa},$$

$\lambda = m\omega^2/4\gamma$, and γ is the force constant in the crystal volume.

The addition to the unperturbed density of states in this spectral region is

$$\delta g = \frac{1}{\pi}\frac{\partial \varphi}{\partial \lambda}. \quad (9)$$

We will calculate it for the symmetric quasilocalized modes. The explicit formulas for φ and $\delta g(\omega)$ are rather cumbersome, so we only present the results of calculations.

The curve for the density of states at a fixed k shows a peak that is slightly shifted from the resonant transmission frequency to lower frequencies. If we are interested in a change in the density of states with changing wave number k along the total transmission curve T (Fig. 2), then we can see that the peak in the density of states near the point at the bulk spectrum edge, where T matches the curve for the dispersion law S of the in-gap localized modes, approaches the total transmission frequency, sharpens with increasing k, and tends to a δ-like shape at the continuum edge (Fig. 3). It is this state that transforms outside the continuum into the symmetric mode localized near the defect (Fig. 2, curve S).

Thus, it is shown by the examples of a 1D quantum system with two groups of excitations and an FCC crystal with a planar defect that the resonant transmission curves in a continuum show peaks of the density of states. The presence of a sharp peak on the curve for the density of vibrational states indicates that the respective vibrations are sharply set off and have resonant character in the continuum. For an FCC crystal, this means that these vibrations may play the role of so-called "leaky waves."

This work was supported in part by the INTAS-1999, grant no. 167.

REFERENCES

1. A. N. Darynskii and G. A. Maugin, Wave Motion **23**, 363 (1996).
2. Ch. S. Kim and A. M. Satanin, Zh. Éksp. Teor. Fiz. **115**, 211 (1999) [JETP **88**, 118 (1999)].
3. A. M. Kosevich, Zh. Éksp. Teor. Fiz. **115**, 306 (1999) [JETP **88**, 168 (1999)].
4. A. M. Kosevich and S. E. Savotchenko, Fiz. Nizk. Temp. **25**, 737 (1999) [Low Temp. Phys. **25**, 550 (1999)].
5. A. M. Kosevich, D. V. Matsokin, and S. E. Savotchenko, Fiz. Nizk. Temp. **25**, 63 (1999) [Low Temp. Phys. **25**, 48 (1999)].

Translated by V. Sakun