SPECIFIC FEATURES OF PARTICLE SCATTERING AND EXCITATION OF QUASILOCAL STATES BY A STATIONARY FLUX IN A TWO-LEVEL SYSTEM

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For a simple model it is demonstrated that the Fano or conventional resonance occurs in systems with a two-level defect depending on the defect parameters. Conditions of the Fano and conventional resonance are analyzed. The problem of a system response to a stationary flux specified on the entire axis by a traveling wave has been solved. It has been found that this flux excites a quasilocal state in the continuous spectrum. Bands of amplitudes of the functions of system response to the stationary flux completely determine the quasilocal state spectrum.

1. In the last few years, there has been an increase in interest in the study of specific features of wave scattering by defects in solid bodies [1, 2]. These specific features are caused by the interaction of the localized states of the discrete spectrum with free waves of the continuous spectrum due to the presence of a defect in the system. Resonance of electrical conductivity caused by the interaction of particles, corresponding to different branches of the spectrum, on the defect was recorded in [3].

The nature of the resonance phenomena in solid bodies is determined by the properties of quasilocal oscillations [4, 5]. The frequencies of such oscillations are within the continuous spectrum. The oscillation density has a clearly defined maximum at the frequency of quasilocal oscillations; therefore, these oscillations are sometimes referred to as resonance ones [6]. Recently it has been demonstrated (see [7]) that long-wave quasilocal oscillations occur in a crystal if the dependence of the frequency on the wave vector is more complex than a quadratic one. It should be remembered that the displacement vector of an elastic wave examined in [1, 2, 4, 5] consists of two independent components (longitudinal and transverse) and the field examined in [7] has a single component (specified by a scalar field). This scalar field is bipartial, that is, it consists of two terms that describe two natural oscillations with different wave vectors but having the same frequencies.

In solid bodies, the characteristics of these waves are specified by a certain set of the parameters. These parameters describe the medium, the wave interaction with the medium and defect, and the interaction of the waves of the same frequencies belonging to different oscillation branches. Resonance of conventional type [7–9] or the Fano resonance [10] occur in the system depending on these parameters.

In the present paper, it is demonstrated that the Fano or conventional resonance occurs at certain values of the parameters characterizing the wave interaction with the defect and the interaction of waves belonging to different brunches of the spectrum.

It is well known that the solution of the scattering problem bears important information on the waves propagating in the crystal and on the defects. In particular, bands of the scattering amplitudes completely determine the discrete spectrum of localized oscillations [11]. We note that the specific features of the continuous spectrum are not manifested in the solution of reference problem on wave scattering by the defect. In the case of a complex law of scattering, information contained in the solution of reference scattering problem is insufficient to derive complete information on the system dynamics. Recall that the standard formulation of the scattering problem implies the presence of incident and reflected waves on one side of the defect and a transmitted wave on the other side of the defect. However, the nonconduction stationary state of the continuous spectrum typical, for example, of the quasilocal state occurs on both sides of the defect throughout the crystal volume. Therefore, the standard formulation of the scattering problem is incomplete. It is assumed that the continuous spectrum of

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quasilocal states can be obtained by solving the problem on system response to a stationary flux specified on the entire axis by a traveling wave.

We now consider this problem for a simple quantum-mechanical one-dimensional model of a two-level system [11]. Let a point defect located at the origin of coordinates $x = 0$ be in the ground state with energy E_g or in the excited state with energy E_e. The defect interaction with an oncoming particle is described by the delta-potential. The Hamiltonian of the examined two-level system includes the kinetic energy of the particle, the energy of elastic scattering by the point defect with intensity σ, and the energy of transition from the ground state to the excited one with intensity β:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + E_g a_g^+ a_g + E_e a_e^+ a_e + \frac{\hbar^2}{2m}\delta(x)\{\alpha(a_g^+ a_g + a_e^+ a_e) + \beta(a_g^+ a_e + a_e^+ a_g)\}, \tag{1}$$

where a_g^+ and a_g are the operators of creation and annihilation of the point defect in the ground state and a_e^+ and a_e are the operators of creation and annihilation in the exited state, respectively. The wave function of the two-level system obeys the Schrödinger equation $H\Psi = E\Psi$ and comprises two terms with the defect in the ground and excited states:

$$\Psi(x) = a_g^+|0\rangle\psi_g(x) + a_e^+|0\rangle\psi_e(x), \tag{2}$$

where the wave functions $\psi_g(x)$ and $\psi_e(x)$ of the ground and excited states are independent solutions of the Schrödinger equation.

After integration of the Schrödinger equation near the point $x = 0$, taking advantage of the orthogonality condition of the ground and excited states, we can easily derive the system of boundary conditions [11]:

$$\begin{cases} \dfrac{d\psi_g(+0)}{dx} - \dfrac{d\psi_g(-0)}{dx} = \alpha\psi_g(0) + \beta\psi_e(0), \\ \dfrac{d\psi_e(+0)}{dx} - \dfrac{d\psi_e(-0)}{dx} = \alpha\psi_e(0) + \beta\psi_g(0). \end{cases} \tag{3}$$

These conditions are supplemented by the continuity condition for the wave functions of the ground and excited states. We note that without interaction (β = 0), the system is separated into independent states $\psi_g(x)$ and $\psi_e(x)$.

2. We first consider the reference problem on particle scattering by the defect for the model described by Eqs. (1)–(3). Let the particle with energy $E_g < E < E_e$ impinge on the defect at $x < 0$. In this case, the particle energy is insufficient to translate the defect into the exited state, and scattering will be elastic. Then the wave functions should be searched in the form

$$\psi_g(x) = \begin{cases} e^{ikx} + Re^{-ikx}, & x < 0, \\ Te^{ikx}, & x > 0, \end{cases} \tag{4}$$

$$\psi_e(x) = M\exp(-\kappa_e|x|), \tag{5}$$

where $k^2 = 2m(E - E_g)/\hbar^2$ and $\kappa_e^2 = 2m(E_e - E)/\hbar^2$. Substituting wave functions (4) and (5) into boundary conditions (3), the corresponding scattering amplitudes

$$R = \frac{i\Delta_R(E)}{\Delta(E)}, \quad T = \frac{\Delta_T(E)}{\Delta(E)}, \quad M = \frac{\Delta_M(E)}{\Delta(E)} \tag{6}$$

can be easily obtained, where

$$\Delta_R(E) = \beta^2 - \alpha(\alpha + 2\kappa_e)\,,\ \Delta_T(E) = 2k(\alpha + 2\kappa_e)\,,\ \Delta_M(E) = -2k\beta\,, \tag{7}$$

$$\Delta(E) = \Delta_T(E) - i\Delta_R(E)\,. \tag{8}$$

The reflection ($|R|^2$) and transmission ($|T|^2$) coefficients have peculiarities which do not manifest themselves in scattering on the simple point defect with the single state (at $\beta = 0$) [8]. For nonzero defect intensity α, the resonance transmission of the particle (when $|R|^2 = 0$ and $|T|^2 = 1$) occurs when

$$\kappa_e^T = (\beta^2 - \alpha^2)/2\alpha\,. \tag{9}$$

The resonance energy of the transmitted particle is

$$E_T = E_e - \frac{\hbar^2\alpha^2}{8m}\left(1 - \frac{\beta^2}{\alpha^2}\right)^2. \tag{10}$$

The wave functions correspond to the localized state $\psi_e(x) = \frac{\alpha}{\beta}\exp\left(-\kappa_e^T|x|\right)$ and to the stationary flux of the free particle in the ground state $\psi_g(x) = \exp\left(ik_T x\right)$, where $k_T^2 = \frac{2m}{\hbar^2}(E_e - E_g) - \frac{\alpha^2}{4}\left(1 - \frac{\beta^2}{\alpha^2}\right)^2$.

The resonance reflection of the particle from the defect (when $|R|^2 = 1$ and $|T|^2 = 0$) occurs when

$$\kappa_e^R = -\alpha/2\,. \tag{11}$$

The resonance reflection energy in this case is

$$E_R = E_e - \frac{\hbar^2\alpha^2}{8m}\,. \tag{12}$$

The standing wave

$$\psi_g(x) = \begin{cases} 2i\sin k_R x, & x < 0\,, \\ 0, & x > 0 \end{cases} \tag{13}$$

arises in the ground state only in the half-space, where $k_R^2 = \frac{2m}{\hbar^2}(E_e - E_g) - \frac{\alpha^2}{4}$, and the wave function of the localized state is $\psi_e(x) = \frac{2k_R}{i\beta}\exp(-\kappa_e^R|x|)$. Solutions of this type were analyzed in [8].

As follows from resonance reflection condition (11), localization of the exited state is necessary in order that the energy of particle interaction with the defect be negative: $\alpha < 0$. Moreover, because the minimum particle energy is equal to the energy of the ground state, there is a threshold value of this parameter $\alpha < \alpha_{\max}$, where $\alpha_{\max} = -2\sqrt{2m(E_e - E_g)/\hbar^2}$ is the maximum intensity of particle interaction with the defect.

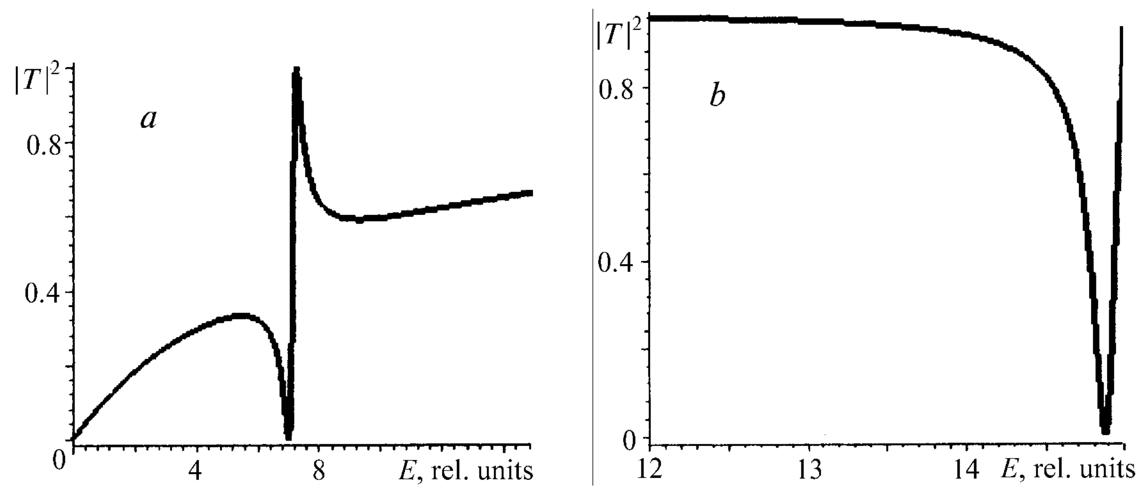

Fig. 1. Dependence of the transmission coefficient $|T|^2$ on the energy for $m = 1$, $E_g = 0$, $E_e = 15$: *a*) $\alpha = -8$ and $\beta = 1$; *b*) $\alpha = -1$ and $\beta = 2$.

If we plot the dependence, for example, of the transmission coefficient $|T|^2$ on the energy E (Fig. 1), we will see that this dependence represents the Fano resonance for certain values of the defect parameters (Fig.1*a*) and the conventional resonance (Fig. 1*b*) for other values of the defect parameters.

In the first case, the total reflection and transmission can be observed at certain values of the parameters. As is well known [10], the resonance transmission and reflection levels are very close for the Fano resonance (Fig. 1*a*), that is, the condition of the Fano resonance $|E_T - E_R| << E_T - E_g$ is satisfied. Therefore, we suggest that the Fano resonance occurs when the energy of particle interaction with the defect exceeds significantly the energy of defect translation into the exited state: $\alpha >> \beta$. This important fact was overlooked in [11].

In the second case, only the total reflection (Fig. 1*b*) occurs. In this case, the condition $E_e - E_R << E_R - E_g$ must be satisfied, that is, the resonance total reflection level must be close to the energy level of the exited state. Conditions of resonance are analyzed in Sec. 5 by calculating the density of the system states.

Following [11], we note that bands of scattering amplitudes (6) determine the discrete spectrum of the system with the defect. Indeed, the determinant of Eq. (7) vanishes only when $k = i\kappa_g$ for $E < E_g$. In this case, the dispersion relation

$$\beta^2 = (\alpha + 2\kappa_g)(\alpha + 2\kappa_e)\,, \tag{14}$$

derived in [11], determines the spectrum of local states $\psi_j(x) = M_j \exp(-\kappa_j|x|)$, where $\kappa_j^2 = 2m(E_j - E)/\hbar^2$ and $j = g, e$.

3. If the particle energy is within the continuous spectrum $E_g < E < E_e$, we will seek for the wave function of the local state in the form of Eq. (5) and the wave function of the ground state in the form

$$\psi_g(x) = \begin{cases} A\cos(kx + \varphi_1), & x < 0\,, \\ B\cos(kx + \varphi_2), & x > 0\,. \end{cases} \tag{15}$$

Substituting solutions of Eqs. (5) and (15) into boundary conditions (3), we obtain the following relation between the phases:

$$\tan\varphi_1 - \tan\varphi_2 = \frac{\alpha(\alpha + 2\kappa_e) - \beta^2}{k(\alpha + 2\kappa_e)}, \tag{16}$$

which specifies the spectrum of nonconduction stationary states. It can be seen that wave function (2) represents superposition of standing wave (15) and state (5) localized near the defect. These states are typical of the continuous spectrum of the system with a defect and are conventionally referred to as quasilocal states [4, 5].

With the point defect, a solution of the Schrödinger equation engendered by Hamiltonian (1) is an even function [11]. If we set $\varphi_1 = -\varphi_2$, we obtain $A = B$, and the solution is

$$\psi_g(x) = \begin{cases} A\cos(kx - \varphi), & x < 0, \\ A\cos(kx + \varphi), & x > 0. \end{cases} \tag{17}$$

The continuous spectrum of even quasilocal states specified by Eq. (17) is determined by the formula

$$\tan\varphi = \frac{\beta^2 - \alpha(\alpha + 2\kappa_e)}{2k(\alpha + 2\kappa_e)}, \tag{18}$$

which relates the phase φ and the particle energy E.

The standing wave (17) exists on the entire axis; however, the curious feature of quasilocal states is that there is an asymmetrical stationary state in which the standing wave is defined only on the semiaxis, but the localized solution exists on both sides of the defect. Indeed, if we set $B = 0$ in Eq. (15), from the boundary conditions it immediately follows that $\varphi_1 = \pi/2 + \pi n$ (where n are integers), that is, $\psi_g(0) = 0$. In this case, the solution obtained from Eq. (15) coincides with Eq. (13), and the condition $\alpha = -2\kappa_e$, which coincides with condition (11) of the resonance particle reflection from the defect, follows from Eq. (16).

4. From an analysis of scattering amplitudes (6) we failed to obtain information on the continuous spectrum of quasilocal states (16). The standard formulation of the scattering problem is somewhat incomplete. Let us explain this statement rewriting solution (4) with allowance for the continuity condition of the wave function of the ground state at point $x = 0$:

$$\psi_g(x) = \begin{cases} (1 + R)e^{ikx} - 2iR\sin kx, & x < 0, \\ (1 + R)e^{ikx}, & x > 0. \end{cases} \tag{19}$$

It then follows that the standard formulation of the scattering problem implies the existence of a certain stationary flux on the entire axis specified by the traveling wave $(1 + R)e^{ikx}$. Now it becomes clear that this formulation of the problem demonstrates the incompleteness of the representation of the sought-for solution by Eq. (19). The second term in Eq. (19) describes the stationary state $2iR\sin kx$ defined only on the semiaxis (x < 0). But we have already demonstrated in Sec. 3 that the quasilocal state exists in the system with a defect not only at $x < 0$ but also at $x > 0$. In this connection, it is of interest to study the dynamics of the examined system for a fixed amplitude of the stationary flux. Then we can seek a complete solution of this problem in the form

$$\psi(x) = Je^{ikx} + \psi_g(x) = \begin{cases} Je^{ikx} + A\cos(kx + \varphi_1), & x < 0, \\ Je^{ikx} + B\cos(kx + \varphi_2), & x > 0. \end{cases} \tag{20}$$

Here solution (15) is taken as a nonconduction state of the continuous spectrum. In our formulation of the problem, we call this solution the system response to a stationary flux. Since the flux amplitude J has been specified, taking advantage of boundary conditions (3), the amplitudes of the response functions can be found:

$$A = J\frac{\Delta_R}{\Delta_\varphi}\cos\varphi_2\,,\ B = J\frac{\Delta_R}{\Delta_\varphi}\cos\varphi_1\,,\ M = J\frac{\Delta_M}{2\Delta_\varphi}\sin(\varphi_2-\varphi_1)\,, \tag{21}$$

where

$$\Delta_\varphi = \frac{\Delta_T}{2}\sin(\varphi_2-\varphi_1) - \Delta_R\cos\varphi_1\cos\varphi_2\,, \tag{22}$$

and Δ_R, Δ_T and Δ_M are determined by Eq. (7).

The poles of response function amplitudes (21) are determined by equating Eq. (22) to zero. They yield dispersion relation (16) for the spectrum of quasilocal states. If we specify one phase, for example, $\varphi_1 = \pi/2$, the stationary flux in the system will excite asymmetrical state (13), and amplitude poles (21) yield condition (11). If we assume that the phases satisfy the relation $\varphi_1 = -\varphi_2$, the stationary flux will excite the even state (17) and the poles of the corresponding amplitudes of response functions will determine the spectrum of quasilocal states (18).

Thus, in our formulation of the problem on the response of the system to the stationary flux, we have succeeded in obtaining solutions describing the resonance features of the reference scattering problem and solutions describing the quasilocal states of the continuous spectrum. This result supplements the well-known conclusions about the specific features of the conventional scattering amplitude and specifies the second method of finding the characteristics of the continuous spectrum of quasilocal states.

5. The scattering relation (18) allows the change in the spectral density of quasilocal states caused by the defect to be calculated from the formula

$$\delta g(E) = \frac{1}{\pi}\frac{d\varphi(E)}{dE} \tag{23}$$

suggested in [12], where the dependence $\varphi(E)$ is specified by Eq. (18). As a result, we obtain the density of states

$$\delta g(E) = \frac{2m}{\pi\hbar^2\kappa_e k}\,\frac{2\alpha k^2\Delta_T(E) + \Delta_R(E)[4k^3 - \kappa_e\Delta_T(E)]}{\Delta_T^2(E) + \Delta_R^2(E)}\,. \tag{24}$$

To determine the resonance condition, the density of states is first expanded into a series around the total reflection energy in powers $E - E_R \ll E_e - E_g$. In this case, the density of states can be written in the form

$$\delta g(E) = \frac{1}{\pi}\frac{\Gamma_R}{\Gamma_R^2 + (E-E_R)^2}\,, \tag{25}$$

where the width of the resonant reflection level is

$$\Gamma_R = -\frac{\hbar^2}{m}\left(\frac{\alpha\beta^2}{4k_R}\right). \tag{26}$$

For resonance occurrence, the condition $\Gamma_R \ll E - E_R < E_e - E_R$ must be satisfied, from which it follows that $\beta^2 \ll |\alpha| k_R$. It can be seen that this condition is satisfied in two cases:

1) the resonance total reflection level is close to the energy of exited state $E_e - E_R \ll E_R - E_g$; this is the case for $|\alpha| < |\beta|$;

2) the energy of particle interaction with the defect exceeds significantly the energy of defect transition into the exited state, that is, $|\beta| << |\alpha|$.

Moreover, as already pointed out in item 2, the intensity of particle interaction with the defect must have the negative sign: $\alpha < 0$.

Now we expand the density of states into a series around the completely transmitted energy in powers $E - E_T << E_e - E_g$. Then the density of states can be written in the form

$$\delta g(E) = \frac{1}{\pi} \frac{\Gamma_T}{\Gamma_T^2 + (E - E_T)^2}, \tag{27}$$

where the width of the resonance transmission level is

$$\Gamma_T = -\frac{2\beta^2}{\alpha^2} \sqrt{(E_e - E_T)(E_T - E_g)}. \tag{28}$$

Resonance occurs when $\Gamma_T << E - E_T < E_e - E_T$. Hence it follows that

$$\left| \frac{2\beta^2}{\alpha^2} \sqrt{\frac{E_T - E_g}{E_e - E_T}} \right| << 1.$$

It can be seen that this condition is satisfied when $|\beta| << |\alpha|$. It turns out that when this condition is satisfied and $\alpha < 0$, total reflection and complete transmission occur for the same set of parameters that satisfy these conditions; moreover, the reflection and transmission levels are close, and Fano resonance occurs. For other parameter values, when the condition $|\alpha| < |\beta|$ is satisfied, only total reflection of the particle from the defect occurs, and the resonance transmission level must be very close to the energy of the ground state, that is, $E_T - E_g << E_e - E_T$.

6. In conclusion it should be noted that the specific features of particle scattering and of the problem of excitation of quasilocal states by a stationary flux examined in the present paper are manifested in systems for which the dispersion curve has at least two branches or the dependence of the energy on the particle momentum is not quadratic. This is the case when the same value of energy corresponds to two (or more) absolute values of the momentum. The waves corresponding to these values of the momentum interact on the defect according to the boundary conditions whose specific form is determined by the corresponding differential equation and the potential of the defect. For the two-level system model examined here, this interaction is characterized by the parameter β. For $\beta = 0$, we have only the particle in the ground state, because $M = 0$. This ground state can be either free or localized, depending on the particle energy.

The quasilocal states, according to the definition, consist of two solutions of different types describing standing waves and solutions localized near the defect. Therefore, these states can be excited by a stationary flux only in systems analogous to those considered in the present paper. As an example, quasilocal acoustic oscillations near a plane defect in a crystal can be mentioned [12] that consist of the standing transverse and localized longitudinal sound waves. The continuous frequency spectrum of these quasilocal oscillations fills the region between the frequencies of the three-dimensional transverse and longitudinal sound waves. A stationary flux of the sound wave in this frequency range, perpendicular to the plane of the defect, will excite quasilocal oscillations in the crystal. The poles of the amplitudes of response functions will determine the continuous spectrum of quasilocal oscillations obtained in [12].

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