Resonance of discrete states against the background of a continuous spectrum

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Interaction of close discrete states against the background of the continuum is considered. In contrast to the known Fano method, the present analysis does not involve a perturbation-theory approximation. A set of nonstationary equations describing the evolution of discrete states against the background of one or several continuums is derived under some relatively general assumptions. The case of two discrete states for a time-independent interaction is investigated in detal and an exact solution is obtained. An analysis of the solution reveals some general regularities of the interaction between discrete levels against the background of a continuum. The evolution of the system is a complicated nonstationary process at an arbitrary magnitude of the interaction between the initial state and the continuum or the finite states of the system evolution. For a certain range of parameters the process becomes quasistationary and the Fano result is a particular case of this regime. New conditions, which have been termed "oscillatory," are realized for another parameter range. When averaged over the oscillation period, these new conditions are found to depend weakly on time. The limits of applicability (with respect to a number of parameters) are determined for both sets of conditions. A number of physical problems illustrating the general results are considered.

1. INTRODUCTION

In many problems of atomic physics it is necessary to consider the interaction between discrete levels and a continuous spectrum. A traditional example of such states against background of a continuum are the auto-ionization levels of atoms. The existence of discrete states leads to the appearance of resonance peaks in the transition probabilities, so that a consideration of the interaction between these levels and the continuum is frequently called resonance theory.

It seems that the main accomplishment in the theory of atomic resonances is the Fano method, which is analogous to the Breit-Wigner method in nuclear physics (see[2], Sec. 142). However, calculations of the transition probability by the Fano method, in spite of their fruitfulness, are limited by perturbation theory in that the initial states are assumed to be weakly coupled to the continuum and to the final states (although the coupling of the final states with the continuum is taken into account exactly). This is most clearly seen in a paper by Kompaneets[3], where the Fano formula was obtained by a nonstationary approach.

In this paper we consider the interaction of discrete states against the background of a continuum in a general formulation that is not connected with perturbation theory. In Secs. 2 and 3 we derive the fundamental system of equations describing the evolution of the states against the background of one or several continums. In Secs. 4 and 5 we investigate in detail, on the basis of an exact solution, the case of two discrete states with stationary interaction. We determine and investigate the limits of appliability applicability of two decay regimes of these states, namely a quasistationary regime (a particular case of which is Fano's result) and an "oscillatory" regime. In Sec. 6 are considered a number of physical problems that illustrate the general results.

2. DISCRETE STATES AGAINST THE BACKGROUND OF ONE CONTINUUM. FUNDAMENTAL SYSTEM OF EQUATIONS

Let

$$\hat{H}=\hat{H}_0+\hat{V}(t),\ \hat{V}(-\infty)=0, \tag{2.1}$$

be the Hamiltonian of a certain quantum system of interacting objects. The spectrum of the unperturbed Hamiltonian H_0 runs through a number of discrete values $\mathscr{E}_n$ and continuous values $\mathscr{E}_\nu$. The discrete states $\{n\}$ lie against the background of the continuous spectrum ν, i.e., there exist $\mathscr{E}_\nu$ such that $\mathscr{E}_n = \mathscr{E}_\nu$.[1)] We assume that the problem of orthogonalization of the wave functions of the continuous spectrum in the absence of an interaction with the discrete spectrum is solved, i.e., we put

$$\langle\nu|H|\nu'\rangle=\mathscr{E}_\nu\delta(\mathscr{E}_\nu-\mathscr{E}_{\nu'}). \tag{2.2}$$

Then the Hamiltonian (2.1) corresponds to the following system of equations for the amplitudes of the states a_n and a_ν:

$$i\hbar\dot{a}_n=\sum_{n'}V_{nn'}\exp(i\omega_{nn'}t)a_{n'}+\int d\nu\, V_{n\nu}\exp(i\omega_{n\nu}t)a_\nu, \tag{2.3a}$$

$$i\hbar\dot{a}_\nu=\sum_{n'}V_{\nu n'}\exp(i\omega_{\nu n'}t)a_{n'}, \tag{2.3b}$$

where $\omega_{\gamma\gamma'} = (\mathscr{E}_\gamma - \mathscr{E}_{\gamma'})/\hbar$ are the frequency of the transitions $\gamma \to \gamma'$.

Under rather general assumptions it is possible to "lower the order" of the system (2.3). For this it is necessary that the distance from the levels $\{n\}$ to the nearest boundary of the continuum $\tilde{\mathscr{E}}$ be large in comparison with the following three quantities: a) the distances between the levels $\hbar\omega_{nn'}$—resonance of the levels; b) the characteristic frequencies $\hbar/\tau$ of the variation of the operator V(t)—adiabaticity of the perturbation; c) the characteristic widths Γ and shifts Δ of the levels $\{n\}$ (see below). These conditions take the form

$$\text{a) } \hbar\omega_{nn'}\ll\tilde{\mathscr{E}},\ \text{b) } \hbar/\tau\ll\tilde{\mathscr{E}},\ \text{c) } \hbar\Gamma, \hbar\Delta\ll\tilde{\mathscr{E}}. \tag{2.4}$$

Then, integrating (2.3b) with respect to time and substituting in (2.3a), we can take the functions $V_{n\nu}(t)$ and $a_n(t)$, which vary slowly in comparison with the oscillating exponentials, outside the sign of integration with respect to t, after which the integration with respect to t yields the ζ function $\zeta(\omega_{n'\nu})$ (cf.[4], p. 164 of the English edition). Proceeding then to integration with respect to dν to $d\mathscr{E} = (d\nu/d\mathscr{E})^{-1}d\nu$ (where $d\nu/d\mathscr{E}$ varies little over the interval $\omega_{nn'}$ far from the boundary of the continuum), we reduce the system (2.3) to the form[2)]

$$i\hbar\dot{a}_n=\sum_{n'}(V_{nn'}-{}^1/_2 iW_{nn'})\exp(i\omega_{nn'}t)a_{n'} \tag{2.5}$$

where

$$W_{nn'}=\Gamma_{nn'}+i\Delta_{nn'},$$
$$\Gamma_{nn'}=2\pi\frac{d\nu}{d\mathscr{E}}V_{n\nu}(t)V_{\nu n'}(t)|_{\mathscr{E}_\nu=\mathscr{E}_n}, \tag{2.6a}$$

$$\Delta_{nn'}=2\,\mathrm{P}\int\limits_{-\infty}^{\infty}\frac{d\mathscr{E}}{\mathscr{E}_n-\mathscr{E}}\frac{d\nu}{d\mathscr{E}}V_{n\nu}(t)V_{\nu n'}(t). \tag{2.6b}$$

Expressions (2.5) constitute the fundamental system of equations describing the resonance of the discrete states against the background of the continuum. The derivation of this system is based only on the condition (2.4); on the other hand, the relations between the quantities $V_{nn'}$, $W_{nn'}$, $\hbar\omega_{nn'}$, and $\hbar/\tau$ can in general be arbitrary. The conditions (2.4) have enabled us to decouple Eqs. (2.3a) and (2.3b), so that the next step in the solution consists of determining the amplitudes a_n from the much simpler system (2.5) and substituting the result in (2.3b).

The interaction with the continuous spectrum has been reduced in (2.5) to a change of the transition matrix in the equations for the amplitudes a_n. This change, however, is of fundamental character and becomes manifest, in particular, in the non-Hermitian character of the transition matrix, leading to nonconservation of the normalization of the amplitudes of the discrete states as a result of their decay into the continuum. The rate $\dot{w}_n$ of this decay can be easily obtained with the aid of (2.5):

$$\dot{w}_n=\frac{d}{dt}|a_n|^2=-\frac{2}{\hbar}\,\mathrm{Im}\sum_{n'}\left(V_{nn'}+\frac{1}{2}\Delta_{nn'}-\frac{i}{2}\Gamma_{nn'}\right)\exp(i\omega_{nn'}t)\,a_n^*a_{n'}. \tag{2.7}$$

Summing (2.7) over n and using the Hermitian character of the matrices $V_{nn'}$ and $\Delta_{nn'}$, we obtain

$$-\dot{w}\equiv\sum_n\dot{w}_n=-\sum_{n,n'}\Gamma_{nn'}\exp(i\omega_{nn'}t)\,a_n^*a_{n'}. \tag{2.8}$$

The quantity $\dot{w}$ is the total rate of the transition from the aggregate of the discrete states $\{n\}$ into the continuum. This can be verified by directly calculating $\dot{w}$:

$$\dot{w}=\frac{d}{dt}\int|a_\nu|^2\,d\nu=\frac{2\pi}{\hbar}\left|\frac{d\nu}{d\mathscr{E}}\sum_n V_{n\nu}\exp\left(\frac{i\mathscr{E}_nt}{\hbar}\right)a_n\right|^2. \tag{2.9}$$

From (2.8) and (2.9) it follows that the normalization of the total wave function, with allowance for the continual states, is conserved.

3. SEVERAL CONTINUUMS. SCATTERING PROBLEMS

Let us generalize the results of Sec. 2 to include the case of several continuums $\{\nu_1, \nu_2, \ldots, \nu_m\}$. In this case the initial system of equations differs from (2.3) only in the presence of additional summation over the continuums m. We note that this notation presupposes orthogonalization of the wave functions not only of each continuum, but also of the different continuums with one another. If the conditions (2.4) are satisfied for $\tilde{\mathscr{E}} = \min\{\tilde{\mathscr{E}}_m\}$, where $\tilde{\mathscr{E}}_m$ is the distance from the levels $\{n\}$ to the boundary of the m-th continuum $\{\nu_m\}$, then relations (2.5)–(2.7) are valid, with

$$\Gamma_{nn'}\equiv\sum_m\Gamma_{nm,mn'}=2\pi\sum_m\frac{d\nu_m}{d\mathscr{E}}V_{n\nu_m}V_{\nu_mn'}\big|_{\mathscr{E}_{\nu_m}=\mathscr{E}_{n'}}, \tag{3.1a}$$

$$\Delta_{nn'}\equiv\sum_m\Delta_{nm,mn'}=\sum_m 2\,\mathrm{P}\int\limits_{-\infty}^{\infty}\frac{d\mathscr{E}}{\mathscr{E}_{n'}-\mathscr{E}}\frac{d\nu_m}{d\mathscr{E}}V_{n\nu_m}V_{\nu_mn'}. \tag{3.1b}$$

We could also introduce the decay rate $\dot{w}_m$ of the states in each of the continuums and the summary rate $\dot{w}$:

$$\dot{w}_m=\sum_{n,n'}\Gamma_{nm,mn'}\exp(i\omega_{nn'}t)\,a_n^*a_{n'},\qquad \dot{w}=\sum_m\dot{w}_m. \tag{3.2a}$$

The analog of formula (2.9) is

$$\dot{w}_m=\frac{2\pi}{\hbar}\left|\frac{d\nu_m}{dE}\sum_n V_{n\nu_m}\exp\left(\frac{i\mathscr{E}_nt}{\hbar}\right)a_n\right|^2, \tag{3.2b}$$

$$|\Gamma_{nm,mn'}|^2=\Gamma_{nm,mn}\Gamma_{n'm,mn'},\qquad |\Gamma_{nn'}|^2\leqslant\Gamma_{nn}\Gamma_{n'n'}, \tag{3.3}$$

the equality in the last formula corresponding to the case of one continuum.

Certain scattering problems can be reduced to the equations obtained above. The scattering problems differ mainly in that the Hamiltonian $\hat{H}_0$ does not have "purely" discrete states in this case, and which are therefore labeled each as states by two subscripts, discrete k and continuous ν, and represent the eigenvalues $\mathscr{E}_{k\nu}$, in the form $\mathscr{E}_{k\nu} = \mathscr{E}_k + \mathscr{E}_\nu$.

We are interested here in a certain limited group of scattering problems connected with the following assumptions. Assume that it is possible to separate from the aggregate of the discrete levels $\{k\}$ a subgroup $\{n\}$ of resonating states, i.e., such that the frequencies of the transitions between them are much lower than the other frequencies: $\omega_{nn'} \ll \omega_{nm}$. Here $\{m\}$ are the remaining nonresonating states from the aggregate $\{k\}$. We assume that the transition between the states of the group $\{n\}$ are not accompanied by changes in the energy of the continuum. Then, solving the elastic-scattering problem, we get

$$\langle n\nu|H|n'\nu'\rangle=V_{nn'}\delta(\nu-\nu').$$

In this case the states $\{n\}$ appear as discrete levels, for which equations of the type (2.3a) are valid, while the change in the index ν is connected with transitions to the "remote" levels $\{m\}$.

Let the system be initially in one of the resonating states $\{n\}$, while the wave function of the continuous spectrum corresponds to a definite state ν_0.[3)] If the matrix elements $V_{n\nu_0,n'\nu'}$ and $V_{n\nu_0,m\nu_m}$ are small in comparison with the transition frequencies ω_{nm}, we can regard the amplitudes $a_{n\nu_0}$ as the principal terms, and the remaining amplitudes $a_{m\nu}$ and $a_{n\nu}$ ($\nu \neq \nu_0$) as correction terms, thus obtaining

$$i\hbar\dot{a}_{m\nu_m}=\sum_{n'}V_{m\nu_m,n'\nu_0}\exp(i\omega_{m\nu_m,n'\nu_0}t)\,a_{n'\nu_0}. \tag{3.4}$$

Further transformations of (3.4) lead, naturally, to expressions (2.5)–(2.7) and (3.1)–(3.3), where a_n should be taken to mean $a_{n\nu_0}$, and $V_{n\nu_m}$ should be taken to mean $V_{n\nu_0,m\nu_m}$. The conditions for the applicability of these expressions coincide with (2.4), where $\tilde{\mathscr{E}}$ stands for the distance to the nearest level of the group $\{m\}$, namely $\tilde{\mathscr{E}} = \min\{\hbar\omega_{nm}\}$. This means, in particular, that the initial wave packet becomes slightly smeared out in comparison with $\tilde{\mathscr{E}}$, thus justifying the formulation (3.4).

4. TWO-LEVEL PROBLEM WITH STATIONARY PERTURBATION. LIMITING CASES

We consider the system (2.5) for two levels, n = 1 and 2, and for a time-independent perturbation V that is instantaneously turned on at t = 0:

$$i\dot{a}_1=-i\gamma_1a_1+(V-i\gamma)e^{i\Delta\omega t}a_2, \tag{4.1a}$$

$$i\dot{a}_2=-i\gamma_2a_2+(V-i\gamma)e^{-i\Delta\omega t}a_1 \tag{4.1b}$$

with initial conditions $a_1(0) = 1$ and $a_2(0) = 0$. We have introduced here the notation

$$\gamma_1=\Gamma_{11}/2\hbar,\ \gamma_2=\Gamma_{22}/2\hbar,\ \gamma=\Gamma_{12}/2\hbar,$$
$$V=V^*=(V_{12}+{}^1\!/_2\Delta_{12})/\hbar,\ \Delta\omega=\omega_{12}+(V_{22}+{}^1\!/_2\Delta_{22}-V_{11}-{}^1\!/_2\Delta_{11})/\hbar,$$

where the quantities $\Gamma_{nn'}$ and $\Delta_{nn'}$ are defined by formulas (2.6) or (3.1). We note that V and γ are real quantities; this is the result of the proper choice of the phases of the discrete wave functions.

Relations (2.7) and (2.8) are rewritten in the form

$$\dot{w}_1=-2(\gamma_1 w_1+\gamma w_{12}),\ \dot{w}_2=-2(\gamma_2 w_2+\gamma w_{12}), \quad (4.2a)$$

$$\dot{w}=2(\gamma_1 w_1+2\gamma w_{12}+\gamma_2 w_2), \quad (4.2b)$$

$$w_{12}=\mathrm{Re}(e^{-i\Delta\omega t}a_1 a_2^*). \quad (4.2c)$$

for the case of one continuum we have $\gamma = (\gamma_1\gamma_2)^{1/2}$ and (4.2b) takes the form

$$\dot{w}=2|\gamma_1^{1/2}a_1+\gamma_2^{1/2}e^{i\Delta\omega t}a_2|^2. \quad (4.3)$$

We consider the limiting cases of the solution of the system (4.1). We shall show that the Fano result follows from (4.1) if perturbation theory is used in terms of the quantity $V - i\gamma$. Putting $a_1 = 1$ in (4.1b), we obtain a_2; then putting a_2 in (4.3) and changing over to sufficiently long times $\gamma_2 t \gg 1$, we arrive at the Fano formula[1]:

$$\dot{w}=2\frac{|\gamma_1^{1/2}\Delta\omega+V\gamma_2^{1/2}|^2}{\Delta\omega^2+\gamma_2^2}. \quad (4.4)$$

It is clear from the derivation that (4.4) is valid under the conditions

$$\gamma_2\gg\gamma_1,\ V;\quad \gamma_2^{-1}\ll t\ll\gamma_1^{-1},\ V^{-1}. \quad (4.5)$$

In essence, the conditions (4.5) are the simplest criteria of a quasistationary regime.

Let us consider the limit that is the converse of perturbation theory, when

$$V\gg\gamma_1,\ \gamma_2;\quad V^{-1}\ll t\ll\gamma_1^{-1},\ \gamma_2^{-1}. \quad (4.6)$$

In this case we can retain in (4.1) only the terms containing V. Then the solutions of (4.1) and the probability (4.3) oscillate rapidly with a frequency $\Omega_0 = (\Delta\omega^2 + 4V^2)^{1/2}$. For such an "oscillatory" regime, physical interest attaches to quantities averaged over the oscillation period $2\pi/\Omega_0$:

$$\bar{w}_1=\frac{\Delta\omega^2+2V^2}{\Delta\omega^2+4V^2},\quad \bar{w}_2=\frac{2V^2}{\Delta\omega^2+4V^2}, \quad (4.7)$$

$$\bar{\dot{w}}=\gamma_1+\frac{|\gamma_1^{1/2}\Delta\omega+\gamma_2^{1/2}\cdot 2V|^2}{\Delta\omega^2+4V^2}. \quad (4.8)$$

Expression (4.8) describes, just as the Fano formula (4.4), a certain resonant interference process. We note that the form of the resonance for (4.4) and (4.8) is determined by the same function

$$f(x)=(x+q)^2/(x^2+1), \quad (4.9)$$

where in the Fano case we have

$$x=\Delta\omega/\gamma_2,\ q=V/\gamma=V/(\gamma_1\gamma_2)^{1/2}$$

and in the case of (4.8) we have

$$x=\Delta\omega/2V,\ q=(\gamma_2/\gamma_1)^{1/2}.$$

The oscillating decay in a two-level system has been studied in considerable detail (see, e.g.,[6]), but the interference effect described by formula (4.9) has not hitherto been analyzed, since the considered problems pertained usually to the case $\gamma = 0$ (see Sec. 6, example 2).

5. ANALYSIS OF THE GENERAL SOLUTION OF THE TWO-LEVEL PROBLEM

Let us turn to the general solution of the system (4.1). Without dwelling on the intermediate calculations, we present the final result

$$a_1=\exp\left(-\frac{\gamma_1+\gamma_2}{2}t+i\frac{\Delta\omega}{2}t\right)\frac{1}{\Omega+i\beta}$$
$$\times\left[\exp\left(\frac{\beta-i\Omega}{2}t\right)\left(\frac{\Delta\omega+\Omega}{2}+i\frac{\gamma_2-\gamma_1+\beta}{2}\right)\right.$$
$$\left.-\exp\left(\frac{-\beta+i\Omega}{2}t\right)\left(\frac{\Delta\omega-\Omega}{2}-i\frac{\gamma_2-\gamma_1-\beta}{2}\right)\right], \quad (5.1a)$$

$$a_2=\exp\left(-\frac{\gamma_1+\gamma_2}{2}t-i\frac{\Delta\omega}{2}t\right)$$
$$\times\frac{V-i\gamma}{\Omega+i\beta}\left(\exp\left(\frac{\beta-i\Omega}{2}t\right)-\exp\left(\frac{-\beta+i\Omega}{2}t\right)\right). \quad (5.1b)$$

Here Ω and β are real numbers defined by the relation

$$\Omega+i\beta=\pm\{[\Delta\omega^2+4V^2-(\gamma_1-\gamma_2)^2]+2i[\Delta\omega(\gamma_2-\gamma_1)-4\gamma V]\}^{1/2}. \quad (5.2)$$

The solution (5.1) depends in a complicated manner on five parameters: $\Delta\omega$, V, γ_1, γ_2, and γ and on the time t. We can verify, however, that in general the time dependences of $|a_{1,2}(t)|^2$ and $\dot{w}(t)$ are of the form

$$e^{-(\gamma_1+\gamma_2)t}(Ae^{-\beta t}+Be^{-i\Omega t}+Ce^{\beta t}), \quad (5.3)$$

where the constants A, B, and C are determined by the parameters $\Delta\omega$, V, γ_1, γ_2, and γ. It is seen from (5.3) that any particular regime is realized simultaneously for all the physical quantities in the corresponding time intervals, depending on the relation between the three parameters $\gamma_1 + \gamma_2$, β, and Ω.

First of all, at any relation between γ_1, γ_2, β, and Ω there is an initial stage of the process, when $t \ll (\gamma_1 + \gamma_2)^{-1}$, β^{-1}, Ω^{-1}. In this case one state a_1 decays into the continuum, as it should:

$$w_1=1,\ w_2=0,\ \dot{w}=2\gamma_1=-\dot{w}_1.$$

If

$$\gamma_1+\gamma_2\gg\gamma_1+\gamma_2\pm\beta,\quad (\gamma_1+\gamma_2)^{-1}\ll t\ll(\gamma_1+\gamma_2\pm\beta)^{-1}, \quad (5.4)$$

then the quasi stationary regime is realized and is characterized by the quantities

$$w_1=\frac{1}{4}\frac{(\Delta\omega\pm\Omega)^2+4\gamma_2^2}{\Omega^2+\beta^2},\quad w_2=\frac{V^2+\gamma^2}{\Omega^2+\beta^2}, \quad (5.5a)$$

$$w_{12}=\frac{1}{2}\frac{V(\Delta\omega\pm\Omega)+2\gamma_2\gamma_1}{\Omega^2+\beta^2}. \quad (5.5b)$$

The other, oscillatory, regime is possible if

$$\Omega\gg\gamma_1+\gamma_2,\quad \Omega^{-1}\ll t\ll(\gamma_2+\gamma_1)^{-1}, \quad (5.6)$$

when the averaged quantities do not depend on the time

$$\bar{w}_1=\frac{1}{2}\frac{\Delta\omega^2+\Omega^2}{\Omega^2},\quad \bar{w}_2=4\frac{V^2+\gamma^2}{\Omega^2}, \quad (5.7a)$$

$$\bar{w}_{12}=\frac{1}{2\Omega}[\Delta\omega V+\gamma(\gamma_2-\gamma_1)]. \quad (5.7b)$$

Let us determine the range of the parameters $\Delta\omega$, V, γ_1, γ_2, and γ in which these regimes are realized. To this end we introduce new variables $\Delta\omega$ and 2V, which are obtained from the old ones $\Delta\omega$ and 2V by rotating the coordinate system through an angle φ defined by the relation (see Fig. 1)

$$\cos\varphi=(\gamma_2-\gamma_1)/\gamma_0,\quad \sin\varphi=-2\gamma/\gamma_0, \quad (5.8)$$

where $\gamma_0 = [(\gamma_2 - \gamma_1)^2 + 4\gamma^2]^{1/2}$. For the quasistationary regime, assuming $\gamma_1 + \gamma_2 \pm \beta \equiv \delta \ll \gamma_1 + \gamma_2$, we obtain with the aid of (5.2)

$$\Delta\bar{\omega}^2\left[1-\frac{\gamma_0}{\gamma_1+\gamma_2}\right]+2\bar{V}^2\leqslant|\delta|(\gamma_1+\gamma_2). \quad (5.9)$$

This is the equation of an ellipse (Fig. 1) with semiaxes

$$a=(\gamma_1+\gamma_2)\left(\frac{\delta}{\gamma_1+\gamma_2-\gamma_0}\right)^{1/2},\quad b=(\delta(\gamma_1+\gamma_2))^{1/2}.$$

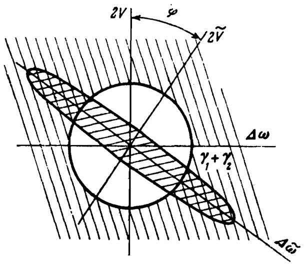

FIG. 1. Regions of realization of the quasistationary and oscillatory regimes $\tan\varphi = -2\gamma/(\gamma_2-\gamma_1)$.

The interior of the ellipse is the region of the quasistationary regime. If $\gamma = (\gamma_1\gamma_2)^{1/2}$, then $\gamma_0 = \gamma_1 + \gamma_2$ and the ellipse degenerates into two straight lines parallel to the $\Delta\omega$ axis (the Fano result corresponds to $\gamma_2 \gg \gamma_1$, V and is valid in a narrow strip near the $\Delta\omega$ axis).

A particularly simple expression is obtained in the quasistationary regime for the probability of the transition to the continuum

$$\dot{w} = \frac{2\gamma_2\tilde{V}^2}{\Delta\tilde{\omega}^2 + (\gamma_1+\gamma_2)^2}. \tag{5.10}$$

This expression generalizes Fano's result to the case of an arbitrary relation between the quantities γ_1, γ_2, and V. If $\gamma_2 \gg \gamma_1$ ($\varphi \to 0$) we arrive at (4.1). The case $\gamma_1 \approx \gamma_2$, which corresponds to the angle $\varphi = \pi/2$, is also of interest. In this case the quantities $\Delta\omega$ and V exchange roles, so that

$$\dot{w} = \frac{1}{\gamma}\frac{|\Delta\omega\gamma + V\Delta\gamma|^2}{(2V)^2+(2\gamma)^2}, \quad \Delta\gamma \equiv \gamma_2-\gamma_1, \quad \Delta\omega \ll 2V, \gamma. \tag{5.11}$$

We proceed to the oscillatory regime. Using expression (5.6), we get from (5.2)

$$\Omega + i\beta = \Omega_0 + i\gamma_0\Delta\omega/\Omega_0.$$

The oscillatory regime is characterized by formulas (5.7), in which we must put $\Omega = \Omega_0$. The decay rates are then calculated from (4.2), with

$$\bar{\dot{w}}_1 = \dot{\bar{w}}_1, \quad \dot{w}_2 = \dot{\bar{w}}_2, \quad \bar{\dot{w}}_{12} = \dot{\bar{w}}_{12}.$$

The regions of the two indicated regimes are plotted in Fig. 1, where the oscillatory regime corresponds to the exterior of the circle with radius $\gamma_1 + \gamma_2$. In the region where the regimes overlap, the corresponding formulas for the probabilities need not necessarily coincide, since these regimes correspond to different observation conditions, as is seen from a comparison of (5.4) with (5.6).

6. CERTAIN EXAMPLES

The theory developed above has certain applications in atomic and possibly nuclear physics. We shall discuss below several concrete physical examples. We are using throughout the concept of a compound object, namely, to reveal the resonating levels we consider not the states of individual objects contained in the quantum system, but the levels of the entire compound system as a whole. The advantage of this approach lies in its consistency, a particularly important factor in complicated cases (see examples 2, 3, and 4).

All the examples considered here are connected with transitions due to the interaction with a monochromatic (e.g., laser) electromagnetic field of intensity

$$E(t) = E_0\cos\omega t. \tag{6.1}$$

These examples make it possible (at least from the fundamental point of view), on the one hand, to trace the continuous transition from a weak perturbation to a strong one by increasing E_0, and on the other hand, to investigate the form of the resonance by varying ω.

Adhering to the concept of a compound object, it is convenient in the analysis of the resonating states to regard the field as a system with a definite number of quanta n_ω, and to include it in the unperturbed Hamiltonian $\hat{H}_0$. In the concrete expressions for the matrix elements, on the other hand, going to the limit as $n \to \infty$, we shall use the quantity E_0.

Example 1 (Fig. 2). Photoeffect under conditions of auto-ionization of an atom (this illustrates the simplest case, the resonance of two discrete states against the background of one continuum).

We assume that the electron shell of the atom X consists of a valence electron e and an atomic residue X^+ with known wave functions. These objects, in conjunction with the electromagnetic field, form the compound system "atomic residue X^+ + electromagnetic field E + valence electron e," the Hamiltonian $\hat{H}$ of which is of the form (2.1), where

$$\hat{H}_0 = \hat{H}_{X^+} + \hat{H}_e + \hat{H}_E, \quad \hat{V} = \hat{V}_{eX^+} + \hat{V}_{EX^+} + \hat{V}_{eE}. \tag{6.2}$$

Let the atomic residue have an isolated excited state $X^+(2)$ with excitation energy $\hbar\omega_0$ exceeding the detachment energy of the valence electron (see Fig. 2a). Let also the frequency ω be close to ω_0. Then the Hamiltonian $\hat{H}_0$ corresponds to two discrete states (Fig. 2b):

$$1 = \{X^+(1),\ n_\omega,\ e_1\}, \quad 2 = \{X^+(2),\ n_\omega - 1,\ e_1\}, \tag{6.3a}$$

that resonate against the background of one continuum

$$\nu = \{X^+(1),\ n_\omega - 1,\ e_\nu\}. \tag{6.3b}$$

Here $X^+(1)$ is the ground state of the atomic residue, while e_1 and e_ν denote the valence electron in the ground and free states, respectively. Thus, we can apply to this problem directly the analysis of Secs. 4 and 5, with the quantities V, γ_1, γ_2 expressed simply in terms of the matrix elements of the operators (6.2). Thus, for example, we have

$$\gamma_1 = {}^1\!/_2\rho(\omega_0)(d_{1\nu}E_0)^2, \quad V^2 = (d_{12}E_0)^2. \tag{6.4}$$

Here $\rho(\omega_0) = 2\pi\hbar^{-1}(d\nu/d\mathscr{E})$, $\mathscr{E} = \hbar\omega_0$ is the density of states of the detached electron.

For this problem, the condition for the validity of the Fano theory (4.6) obviously reduces to a limitation on the field intensity:

$$E_0^2 \ll \frac{\rho(\omega_0)|V_{eX^+}|^2}{2d_{12}^2 + \rho(\omega_0)(d_{1\nu})^2} \equiv E_{cr}^2. \tag{6.5}$$

A deviation from the Fano formula should be observed in fields E_0 that are comparable with (or larger than) the critical field E_{cr}. Let us estimate the value of E_{cr}. If the parameter γ is determined by the electrostatic interaction of the valence electron with the atomic residue then usually (see, e.g.,[7]) $\gamma_2 \sim 10^{-2}$ eV and we have $E_{cr} \sim 10^{-2}$ a.u. $\sim 10^8$ V/cm, i.e., the Fano formula is valid for most real cases. There exist, however, auto-ionization states with large lifetimes, which

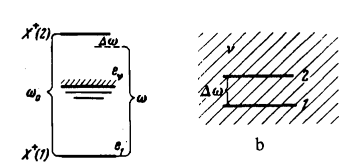

FIG. 2. Photoeffect under conditions of autoionization of the atom (Example 1).

a b

decay either radiatively or (slower still by a factor $\hbar c/e^2$) as a result of spin interaction ([7], p. 249). For these states, the case $E_0 > E_{cr}$ can be frequently realized.

It is most convenient to investigate the shape of the resonance curve in the photoeffect with the aid of tunable lasers. No such lasers have been developed so far for the short-wave region corresponding to excitation of auto-ionization levels of atoms. There is, however, a situation that is favorable from this point of view in the case of negative ions, where the auto-ionization levels are already quite low.

Example 2. Induced transition between spontaneously decaying states of an atom (the monochromatic field is regarded as a discrete object, and the spontaneous field is continuums).

States 1 and 2 of the atom X, coupled by the field (6.1), decay spontaneously into other states X(m). Here $H_0 = H_X + H_E + H_{vac}$ (where H_{vac} is the Hamiltonian of the zero-point oscillations of the field) has the following discrete states:

$$1=\{X(1), n_\omega, \ldots, n_{\omega_{1m}}, n_{\omega_{2m}}, \ldots\}, \quad 2=\{X(2), n_\omega-1, \ldots, n_{\omega_{1m}}, n_{\omega_{2m}}, \ldots\},$$

which resonate against the background of the continuums that are characterized by the states of the atom X(m) and of the field (6.1), and by the photon occupation numbers:

$$\nu_{1m}=\{X(m), n_\omega, \ldots, n_{\omega_{1m}}+1, n_{\omega_{2m}} \ldots\}, \quad \nu_{2m}=\{X(2), n_\omega-1, \ldots, n_{\omega_{1m}}, n_{\omega_{2m}}+1, \ldots\}.$$

The transitions $1 \to \nu_{1m}$ and $2 \to \nu_{2m}$ correspond to spontaneous transition from the states X(1) and X(2) to the states X(m). We note that the transitions $1 \to \nu_{2m}$ and $2 \to \nu_{1m}$ are forbidden, since they correspond to a simultaneous change of the states of three pairwise interacting objects. Each state interacts only with "its own" continuums, thus, corresponding to the case $\gamma_1\gamma_2 \neq \gamma^2 = 0$. Expressions for γ_1, γ_2, and V are widely known. This problem was considered in detail for weak and strong fields[4,6].

Example 3 (Fig. 3). Ionization and pairwise excitation of atoms in the course of a collision in a radiation field (radiative collision; it illustrates the more complicated case of resonance against the background of two continuums with a time-dependent interaction).

The atoms X and Y collide in the field (6.1), and the energy is close to the sum of the excitation energies of the atoms, $\hbar\omega_0 = \mathscr{E}_{21}^X + \mathscr{E}_{21}^Y$ and exceeds the ionization energy of each of the atoms. In this case the compound object is "atom X + atom Y + electromagnetic field E." The Hamiltonian is

$$\hat{H}_0=\hat{H}_X+\hat{H}_Y+\hat{H}_E, \quad \hat{V}(t)=\hat{V}_{XY}(t)+\hat{V}_{XE}+\hat{V}_{YE}.$$

In this problem, two discrete states of the unperturbed Hamiltonian H_0 (see Fig. 3b)

$$1=\{X(1), Y(1), n_\omega\}, \quad 2=\{X(2), Y(2), n_\omega-1\},$$

resonate against the background of two continuums

$$\nu_1=\{X(\nu), Y(1), n_\omega-1\}, \quad \nu_2=\{X(1), Y(\nu), n_\omega-1\}.$$

The interaction of the atoms V_{XY} depends parametrically on the distance between the nuclei and consequantly on the time. The transitions $1 \to \nu_1$ and $1 \to \nu_2$ correspond to atom photoionization reactions; the transition $1 \to 2$, which corresponds to excitation of a pair of interacting atoms (quasimolecule) by one

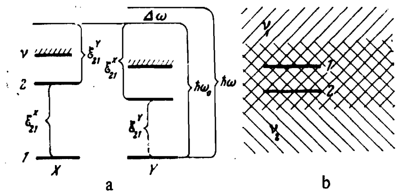

FIG. 3

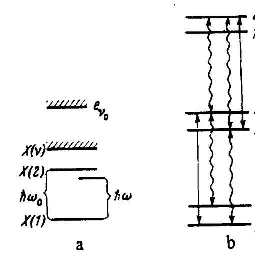

FIG. 4

FIG. 3. Pairwise excitation of atoms with ionization by collision in a radiation field (example 3).

FIG. 4. Scattering of an electron by an atom situated in a resonant electromagnetic field (example 4).

photon is a radiative-collision reaction (analogous to that considered in[8]; the transitions $2 \to \nu_1$ and $2 \to \nu_2$ comprise the reaction of collision ionization of one atom as a result of de-excitation of the other (analogous to the Penning effect, see[7], p. 100).

Example 4 (Fig. 4). Scattering of an electron by an atom situated in a resonant electromagnetic field (illustrates the application of the theory to scattering problems).

The atom (or molecule) X is situated in a field (6.1) whose frequency is close to the frequency ω_0 of the transition $X(1) \to X(2)$. An electron is scattered by the atom. Interest attaches to excitation of the atom by an electron with participation of an optical quantum[4)].

The chosen compound system is "atom X + electromagnetic field E + free electron":

$$\hat{H}_0=\hat{H}_X+\hat{H}_E+\hat{H}_e, \quad \hat{V}=\hat{V}_{XE}+\hat{V}_{eX}+\hat{V}_{eE}.$$

In accordance with the approach developed in Sec. 3 for scattering problems, we find for the object "atom X + field E," which has discrete levels, an aggregate of state $\{n\}$, from which we separate subgroups of resonating states $\{n\}$ and states $\{m\}$ that are far from them. If we exclude two-photon transition from consideration, then we can confine ourselves to the following six discrete states:

$$1=\{X(1), n_\omega\}, \quad 2=\{X(2), n_\omega-1\},$$
$$1'=\{X(1), n_\omega-1\}, \quad 2'=\{X(2), n_\omega-2\},$$
$$1''=\{X(1), n_\omega+1\}, \quad 2''=\{X(2), n_\omega\},$$

of which 1 and 2 form the subgroup $\{n\}$. Figure 4b shows the possible transitions from the states 1 and 2 to the states $1'$, $2'$, $1''$, $2''$ which form the subgroup $\{m\}$. These transitions (to the "remote" levels) are accompanied by corresponding changes in the free-electron energy. On the other hand, transitions within the group of states $\{1, 2\}$, $\{1', 2'\}$, $\{1'', 2''\}$ can be regarded as elastic. The latter makes it possible to reduce the solution of this problem to the general results (3.4) of Sec. 3 for the scattering problems. We note that the considered process of excitation of the atom by the electrons in the presence of an optical field is possible, as a result of interference between a bremsstrahlung transition with a collision transition, as a consequence of the virtual transitions $1 \to 1' \to 2$ or $1 \to 2'' \to 2$ (Fig. 4b). In this connection, the results of[9], where the indicated process is calculated without allowance for bremsstrahlung transitions, seem to need refinement.

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[1)] We note that this situation is possible, inasmuch as $\mathscr{E}_n$ and $\mathscr{E}_\nu$ pertain to an aggregate of objects. For a more complete clarification of the situation, the reader can proceed directly to the concrete examples in Sec. 6.

[2)] The system (2.5) at $\Delta_{nn'} = 0$ was cited in a paper by one of us [5] without proof.

[3)] The corresponding choice of the wave functions of the continuous spectrum is frequently referred to in scattering theory as the formation of a wave packet.

[4)] Transitions of this type were investigated by Hahn and Hertel [9].

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