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# Fano effect studied with use of the recursion method

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We treat the classical problem of a number of discrete states interacting with continua (Fano effect), by means of the recursion method. We first map a continuum of states on an equivalent semi-infinite linear chain; then we take advantage of the concepts and properties of the interaction and dipole carrying states to calculate the absorption spectrum. Our approach leads to a significant simplification of calculations without introducing approximations to the original problem. As an example, we consider the case of discrete states interacting with a semielliptical band: we show that resonances, antiresonances, and narrowing of levels, due to interference effects among interacting channels, can be handled in a very compact and simple way.

## I. INTRODUCTION

The interaction of one or more discrete levels with a continuum of states is a long lasting problem in physics. It was originally studied by Fano[1] in 1935, and later reconsidered by the same author[1] within the Green's-function formalism. The most peculiar feature of the problem is the occurrence of anomalous line shapes in absorption experiments, known as Fano profiles. Examples of Fano profiles are countless in atomic, molecular, and solid-state physics. Perhaps one of the earliest and best known examples is the autoionization of the ultraviolet and core excitations in rare-gas atoms[2] and later in rare-gas solids;[3] for rare-gas solids in particular, use of synchrotron radiation has greatly contributed to further enrich the phenomenology. Also in molecules such profiles have been observed in absorption or predissociation.[4] Among the numerous other problems which can be mimicked with discrete levels interfering with a continuum of states, we can mention resonant impurity levels in crystals,[5,6] discrete excitonic states coupled with continuum states belonging to other excitonic series,[7,8] discrete phonon lines coupled to a phonon quasicontinuum,[9] and hybridization effects in the electronic structure of transition metals and alloys.[10] More recently, the possibility of laser action, without population inversion, involving the pumping of an autoionizing state has attracted considerable attention,[11] even if some previous study[12] anticipated these ideas; at this regard, quantum wells in appropriate semiconductor heterostructures have been recently proposed for experiments.[13]

From a theoretical point of view, the anomalous line shapes arising from interference of discrete levels with a continuum of states can be studied with different approaches, depending on how the continuum of states is handled in the actual physical problem. A possible approach is discretization of the continuum of states by embedding the system in a sufficiently large box; discrete and discretized states are then handled on the same foot[8,14] by means of appropriate numerical diagonalization. The analytic approach, on the other side, treats the continuum of states by means of the Green's-function technique, along the lines laid down by Fano.[1] The advantage of this line of approach, that focuses on analytic aspects rather than on purely numerical ones, is to provide simple expressions for absorption line shapes in simplified though significant situations. This is very useful for an understanding of the key aspects of the problems and for guidelines before considering laborious numerical approaches.

It is interesting to note that the essential difference between the Fano formulations[1] of 1935 and 1961 lies in the adoption of Green's-function techniques available in the interim. Since then, however, several powerful techniques have appeared in the literature for efficient calculations of Green's functions. Among them, the iterative procedure based on the renormalization method[15,16] and the recursion method[17] are of particular value. The physical and technical aspects of the recursion method,[17] as well as its relationship with other iterative methods such as the moment method, the memory function method, and the renormalization approach are by now well established.[16,18,19] The purpose of this paper is a reformulation of the Fano problem exploiting some powerful concept and techniques of the recursion and renormalization methods. We show that this task can indeed be achieved through an appropriate implementation of ideas and procedures of these iterative approaches, leading to elegant and easily interpretable results.

The general treatment of a number of discrete states interacting with a continuum is discussed in Sec. II. There we use the recursion method in a quite unconventional form, to transform a set of orthogonal states into a much more manageable chain structure, the first state of each chain being the "interaction carrying state." In Sec. III we study some interesting exemplifications; for simplicity a model structure is taken for the continuum so we produce a number of simple formulas containing the relevant physics of the multiple interferences between discrete states and a continuum; the mechanism of the narrowing of lines is also presented in a very transparent way. Section IV contains the conclusions.

## II. PROCESSING DISCRETE AND CONTINUUM CHANNELS BY THE RECURSION METHOD

### A. Basic principles and technical aspects

In a number of electronic, excitonic, or vibrational problems of solids, molecules, or atoms, the actual stationary states may be represented by a superposition of states corresponding to discrete and continuous spectra. The more general system under investigation can thus be schematized as composed by one or more discrete levels interacting with one or more continuum channels. In this section we show how to handle this problems with an appropriate implementation of the recursion method; in essence the basic techniques here employed include the use of the recursion method for tridiagonalization of the continuum channels, and the concept and properties of what we call the interaction carrying states. We begin to illustrate our procedure in the case of one discrete state interacting with one continuum.

The Hamiltonian which describes a discrete state $|\Phi_e\rangle$ of energy $E_e$ interacting with a large number $N$ of quasicontinuum states $|\Phi_i\rangle$ of energy $E_i$ can be written as

$$H=E_e|\Phi_e\rangle\langle\Phi_e|+\sum_{i=1}^{N}E_i|\Phi_i\rangle\langle\Phi_i| + \sum_{i=1}^{N}\left[V_{ei}|\Phi_e\rangle\langle\Phi_i|+V_{ei}^{*}|\phi_i\rangle\langle\Phi_e|\right] \tag{1}$$

(where $N$ is the number of states we use to represent the continuum). Such an Hamiltonian is represented schematically in Fig. 1(a). Our purpose is to study the absorption line shape due to the dipole coupling of the ground state $|\Phi_g\rangle$, of energy $E_g$, to the excited state $|\Phi_e\rangle$ and to the continuum channel.

It is evident that the basic obstacle we encounter in dealing with the Hamiltonian (1) is the large (or infinite) number of degrees of freedom of the continuum. These can be conveniently taken into account with a procedure based on the recursion method which selects a seed state and hierarchically orders all the other degrees of freedom. Although the general principles[17,18] of these methods are known, much care and attention must be paid to arrive at something useful.

Let us consider in fact the part of the Hamiltonian (1) corresponding to the band continuum

$$H_c=\sum_{i=1}^{N}E_i|\Phi_i\rangle\langle\Phi_i| . \tag{2}$$

We can choose any initial state,

$$|u_0\rangle=\sum_{i=1}^{N}c_i|\Phi_i\rangle , \tag{3}$$

and transform the diagonal operator $H_c$ into a convenient tridiagonal chain form. According to the standard recursion scheme we apply the following procedure:

$$\begin{aligned}
&|f_0\rangle=|u_0\rangle ,\\
&a_0=\langle f_0|H_c|f_0\rangle ,\\
&|F_{n+1}\rangle=(H_c-a_n)|f_n\rangle-b_n|f_{n-1}\rangle ,\\
&b_{n+1}^2=\langle F_{n+1}|F_{n+1}\rangle ,\\
&|f_{n+1}\rangle=\frac{1}{b_{n+1}}|F_{n+1}\rangle ,\\
&a_{n+1}=\langle f_{n+1}|H_c|f_{n+1}\rangle .
\end{aligned} \tag{4}$$

$H_c$ is tridiagonal on the orthonormal basis $\{|f_n\rangle\}$, and thus the original band is exactly mapped onto a linear semi-infinite chain ($N\rightarrow\infty$).

The arbitrariness in the choice of the seed state of Eq. (3) can be conveniently exploited to simplify the expression of the interaction part of the Hamiltonian (1)

$$H_I=\sum_{i=1}^{N}(V_{ei}|\Phi_e\rangle\langle\Phi_i|+V_{ei}^{*}|\Phi_i\rangle\langle\Phi_e|) \tag{5}$$

on the new basis functions $\{|f_n\rangle\}$. In analogy to the concepts of dipole carrying states,[19] we here introduce the "interaction carrying state" defined as

$$V|f_0\rangle=\sum_{i=1}^{N}V_{ie}|\Phi_i\rangle , \tag{6}$$

where $V$ is such that $|f_0\rangle$ is normalized to one.

If we perform the recursion procedure starting from the interaction carrying state (6), the total Hamiltonian is represented by a one-dimensional chain in which the first state is just the discrete state itself, the second one is the interaction carrying state, and the others are the states of the hierarchy generated by Eqs. (4). That is, the Hamiltonian (1) in the new basis is written as

$$H=E_e|\Phi_e\rangle\langle\Phi_e|+(V|f_0\rangle\langle\Phi_e|+V^{*}|\Phi_e\rangle\langle f_0|) + \sum_{n=0}^{N}a_n|f_n\rangle\langle f_n| + \sum_{n=0}^{N-1}b_{n+1}(|f_{n+1}\rangle\langle f_n|+|f_n\rangle\langle f_{n+1}|) , \tag{7}$$

and the relative pictorial diagram is shown in Fig. 1(b).

To prove the tridiagonal form of Eq. (7), we have to show that

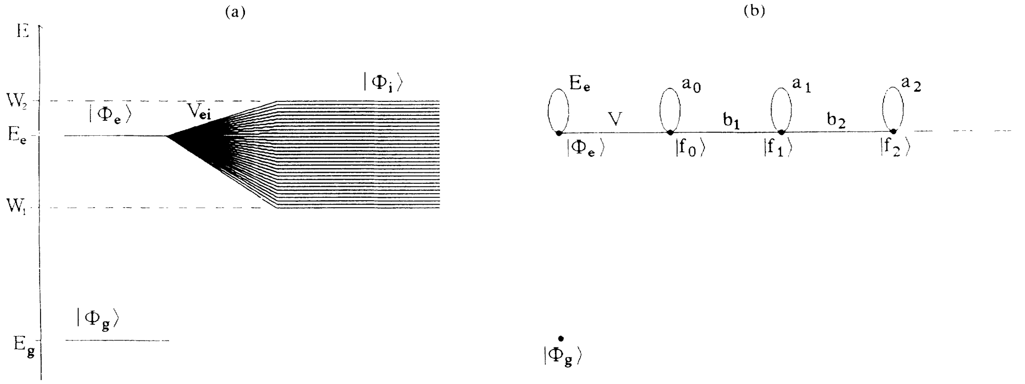

FIG. 1. Schematic representation of a system with a single discrete state $|\Phi_e\rangle$ interacting with a continuum of states $|\Phi_i\rangle$; the edges of the continuum are $W_1$ and $W_2$; $|\Phi_g\rangle$ is the ground state of the system. In (b) the continuum is represented in the equivalent hierarchical basis $|f_n\rangle$ generated by the recursion method. The state $|f_0\rangle$ is the "interaction carrying state," i.e., the state through which all the interactions between the discrete state and the continuum take place.

$$\langle f_n|H|\Phi_e\rangle=0$$

for every $n\neq 0$; this is easily seen if we consider that using the Hamiltonian (1) we obtain

$$\langle f_n|H|\Phi_e\rangle=\sum_{i=1}^{N}\langle f_n|\Phi_i\rangle\langle\Phi_i|H|\Phi_e\rangle=\sum_{i=1}^{N}\langle f_n|\Phi_i\rangle V_{ie}.$$

Because of the definition (6) for the interaction carrying state, we have

$$\langle f_n|H|\Phi_e\rangle=V\sum_{i=1}^{N}\langle f_n|\Phi_i\rangle\langle\Phi_i|f_0\rangle=0\ .$$

Finally, in the same way

$$\begin{aligned}\langle f_0|H|\Phi_e\rangle&=\sum_{i=1}^{N}\langle f_0|\Phi_i\rangle V_{ie}\\&=V\sum_{i=1}^{N}\langle f_0|\Phi_i\rangle\langle\Phi_i|f_0\rangle=V\ ,\end{aligned}$$

and this completes the demonstration of expression (7).

### B. Simplifications and generalizations

The elegant reduction of the Hamiltonian (1) into the chain model (7) is quite general and manageable; it is well suited both for simplifications or for generalizations depending on the specific problems to be handled. Let us consider, for instance, the situation in which the interaction coefficients $V_{ei}$ in $H$ are approximately energy independent in a given energy range (say, $-W, W$) and are negligible outside it; let us denote by $D(E)$ the density of states of the continuum channel. In this case it is easily seen that the coefficients $a_n$ and $b_n$ in the Hamiltonian (7) [obtained by the recursion procedure summarized in Eqs. (4)] coincide with the continued fraction coefficients corresponding to the density of states $D(E)$.

We can choose a band shape with known continued fraction coefficients in order to obtain simple formulas for the self-energy and the Green's function. In the case of semielliptic density of states, for instance, we have

$$D(E)=\frac{2}{\pi W^2}\sqrt{W^2-E^2}\ \text{ for } |E|\le W\ . \tag{8}$$

The coefficients of the corresponding continued fraction are constant and are given by

$$a_n=0\ ,\quad b_n^2=\frac{W^2}{4}\ ,$$

and the Green's function on the initial state $|f_0\rangle$ is (we use the complex notation for the energy $z=E+i\epsilon$)

$$G_{00}(z)=\frac{2}{W^2}(z-i\sqrt{W^2-z^2})\ , \tag{9}$$

where the square root is defined with the cut of the complex plane in $(-\infty,0)$ and the determination $\sqrt{1}=1$.

In the case of a rectangular density of states

$$D(E)=\frac{1}{2W}\ \text{ for } |E|\le W \tag{10}$$

we have instead

$$a_n=0,\quad b_n^2=\frac{n^2W^2}{4n^2+1}\ ,$$

and correspondingly

$$G_{00}(z)=\frac{1}{2W}\ln\left[\frac{z+W}{z-W}\right]\ , \tag{11}$$

where the logarithm is defined with the cut in $(-\infty,0)$ of the complex plane and with the determination $\ln 1=0$.

Suppose now that the interaction coefficients $V_{ei}$ are not constant throughout the channel, although we can separate different regions of the energy spectrum in which they are approximately constant. For each of

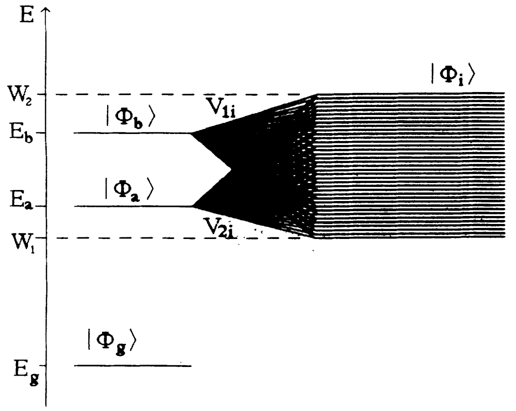

FIG. 2. Schematic representation of a system with two discrete states interacting with a continuum of states $|\Phi_i\rangle$.

these regions we can choose the appropriate interaction carrying state and apply the scheme outlined before. We arrive thus to an equivalent multichain Hamiltonian containing the original discrete state interacting with the first states of a number of chains. It can also be observed that smooth energy dependence of the interaction parameters $V_{ei}$ can be taken into account, whenever necessary, with expansion in Taylor series: each term of the series extends correspondingly the range of the interaction to further steps of the chain representation of the continuum.

If there are several discrete states interacting with a continuum (see for instance Fig. 2) it is evident that our procedure is straightforwardly generalizable. In fact we can consider separately regions of continuum having nearly constant interactions with all discrete states; the equivalent Hamiltonian includes, besides discrete states, an appropriate number of semi-infinite chains on which the continuum has been mapped on. Finally, we can further reduce all the semi-infinite chains with the renormalization procedure and *arrive to a problem with a number of degrees of freedom equal to the number of discrete states plus the number of interaction carrying states considered.* These considerations clearly show how flexible is the present procedure both in handling realistic problems and in working out significant models.

### C. Calculation of the absorption line shape

The usefulness of the chain transformation presented in Sec. II A is further corroborated by the following simple procedure for the calculation of the absorption line shape. Basically we do not have to diagonalize the Hamiltonian but simply to calculate appropriate Green's functions.

Consider in fact the Hamiltonian (1) or the equivalent Hamiltonian (7). The standard expression for the transition probability for unit time from the fundamental state $|\Phi_g\rangle$ to the states $|\varphi_i\rangle$, eigenstates of the Hamiltonian, is given by the Fermi golden rule

$$P_{\varphi_i\leftarrow\Phi_g}=\frac{2\pi}{\hbar}|\langle\varphi_i|T|\Phi_g\rangle|^2\delta(E_i-E_g-\hbar\omega)\ ,$$

where $T$ is essentially the dipole operator, and $E_g$ and $E_i$ are the eigenvalues of $|\Phi_g\rangle$ and $|\varphi_i\rangle$, respectively. The absorption spectrum is proportional to

$$I(\omega)=\sum_i\langle\Phi_g|T|\varphi_i\rangle\langle\varphi_i|T|\Phi_g\rangle\delta(E_i-E_g-\hbar\omega)\ .$$

Similarly to what was done in Ref. 19, let us introduce the dipole carrying state

$$|\chi\rangle=T|\Phi_g\rangle=\sum_i\langle\varphi_i|T|\Phi_g\rangle|\varphi_i\rangle\ . \tag{12}$$

Then the line shape $I(\omega)$ takes the simple form

$$I(\omega)=\sum_i|\langle\chi|\varphi_i\rangle|^2\delta(E_i-E_g-\hbar\omega)$$
$$\equiv n_\chi(\hbar\omega+E_g)=-\frac{1}{\pi}\lim_{\epsilon\to0^+}\mathrm{Im}G_{\chi\chi}(\hbar\omega+E_g+i\epsilon)\ , \tag{13}$$

where $n_\chi(\hbar\omega+E_g)$ is the density of states of the Hamiltonian projected on the dipole carrying state $|\chi\rangle$.

In the case of one excited discrete state $|\Phi_e\rangle$ interacting with a continuum, when both the interactions $V_{ei}$ and the dipole moment matrix elements from the ground state to the continuum states are constant, it is easy to see that the dipole carrying state (12) is a linear combination of the discrete and interaction carrying state

$$|\chi\rangle=T_e|\Phi_e\rangle+T_0|f_0\rangle\ , \tag{14}$$

where $T_e$ and $T_0$ are the dipole moment matrix elements to the discrete excited state and to the interaction carrying state.

In the general case of several discrete states interacting with one or more continua, it is clear that processing separate energy regions of each continuum where both the matrix elements $V_{ei}$ and the dipole operator matrix elements are approximately constant, we recover the situation noted above in which the discrete states interact with several chains only through their first states, with the further advantage that only these states and the discrete states are connected to the ground state by the dipole operator. It is now possible to construct the dipole carrying state as the linear combination of the discrete states and the first states of the chains with coefficients proportional to the respective dipole moments.

With the renormalization procedure we can then process the (noninteracting) semi-infinite chains and reduce ourself to a manageable problem with a relatively small number of degrees of freedom; the needed Green's-function matrix element $G_{\chi\chi}(E)$ is then obtained without difficulty by direct inversion of an appropriate matrix of relatively small rank.

## III. ILLUSTRATIVE EXAMPLES

In this section we show the potentialities of our method by considering a few exemplifications. We consider here simple models for the density of states of the continuum; this allows us to establish analytic solutions and better emphasize relevant physical aspects.

We consider first the case of only one discrete state interacting with one continuum in a given range of energy, as schematized in Fig. 1, with constant interaction matrix elements and dipole matrix elements in the range $(-W,W)$. The normalized dipole carrying state $|\chi\rangle$ is

$$|\chi\rangle=\frac{1}{\sqrt{|T_e|^2+|T_0|^2}}(T_e|\Phi_e\rangle+T_0|f_0\rangle)$$

$$=\tilde{T}_e|\Phi_e\rangle+\tilde{T}_0|f_0\rangle\ ,$$

where we have indicated with $\tilde{T}_e$ and $\tilde{T}_0$ the normalized dipole moment matrix elements from the ground state to the discrete state and to the interaction carrying state, respectively.

With the renormalization procedure we can systematically eliminate all the states $|f_1\rangle,|f_2\rangle,\ldots,|f_n\rangle,\ldots$ of the semi-infinite chain provided the self-energy $\sum(E)$ is evaluated, for the state $|f_0\rangle$, in terms of the recurrence parameters

$$\sum(E)=\cfrac{b_1^2}{E-a_1-\cfrac{b_2^2}{E-a_2-\ddots}}\ .$$

The effective Hamiltonian is now a $2\times2$ matrix (energy dependent) in the space spanned by $|\Phi_e\rangle$ and $|f_0\rangle$, and to obtain the absorption spectrum we only have to calculate its Green's function on the dipole carrying state

$$G_{\chi\chi}(E)=\left\langle\chi\left|\frac{1}{E-H_{\text{eff}}(E)}\right|\chi\right\rangle\ .$$

The explicit expression of the absorption line shape is thus (for $|E|\le W$)

$$n_\chi(E)=-\frac{1}{\pi}\frac{|\tilde{T}_0|^2(E-E_e)^2+(V\tilde{T}_e^*\tilde{T}_0+V^*\tilde{T}_e\tilde{T}_0^*)(E-E_e)+|\tilde{T}_e|^2|V|^2}{\left[\left[\text{Im}\sum(E)\right]^2+\left[E-a_0-\text{Re}\sum(E)\right]^2\right](E-E_e)^2-2|V|^2\left[E-a_0-\text{Re}\sum(E)\right](E-E_e)+|V|^4}\text{Im}\sum(E). \tag{15}$$

[For the sake of precision, the expression (15) of the density $n_\chi(E)$ holds inside the range $(-W,W)$; if $|V|$ is greater than an energy of the order of $W$, one or two discrete states separate from the continuum.]

For simplicity (and also to avoid spurious asymmetry in the absorption due to the actual shape of the continuum relative to the energy $E_e$), we take a symmetric density of states (semielliptic), whose Green's function is given by Eq. (9) and whose self-energy is

$$\sum(E)=\frac{E}{2}-i\frac{1}{2}\sqrt{W^2-E^2}\ ,$$

and choose the discrete state in the middle of the band (i.e., $E_e=0$). Moreover, the interaction $V$ between the discrete state and the continuum is chosen such that $|V|\ll W$. Equation (15) assumes now the simpler form (consider also that $a_0=0$)

$$n_\chi(E)=\frac{|\tilde{T}_0|^2E^2+(V\tilde{T}_e^*\tilde{T}_0+V^*\tilde{T}_e\tilde{T}_0^*)E+|\tilde{T}_e|^2|V|^2}{E^2+\Delta^2}\times\left[\frac{2}{\pi W^2}\sqrt{W^2-E^2}\right]\ , \tag{16}$$

where

$$\Delta=\frac{2|V|^2}{W}\ . \tag{17}$$

We now consider the three illustrative cases shown in Fig. 3, and for each of them we report the absorption spectrum of Eq. (16), taking in any case $V$ equal to one tenth of the bandwidth.

In the case of Fig. 3(a) only the discrete state is dipole connected to the fundamental state (i.e., $\tilde{T}_e=1,\tilde{T}_0=0$); and the presence of the continuum causes the broadening of the absorption peak. In this case Eq. (16) becomes

$$n_\chi(E)=\frac{|V|^2}{E^2+\Delta^2}\left[\frac{2}{\pi W^2}\sqrt{W^2-E^2}\right]\ , \tag{18a}$$

with the typical form of a Lorentzian centered at $E=0$ and broadening value $\Delta=2|V|^2/W$ [see Fig. 3(a)]. In this case the discrete state autoionizes with the continuum states lying at approximately the same energy.

In the case of Fig. 3(b) only the states of the continuum are connected to the fundamental state (i.e., $\tilde{T}_e=0$, $\tilde{T}_0=1$), and Eq. (16) reduces to

$$n_\chi(E)=\left[1-\frac{\Delta^2}{E^2+\Delta^2}\right]\left[\frac{2}{\pi W^2}\sqrt{W^2-E^2}\right]\ . \tag{18b}$$

We see in Fig. 3(b) that the presence of the discrete state causes a hole of half-width $\Delta$ (it is a level repulsion mechanism). In this case the absorption is proportional to the perturbed density of states. We may interpret the results of Fig. 3(b) as follows: the presence of the discrete state $|\Phi_e\rangle$ of energy $E_e$ gives rise to a perturbed density of states depleted at $E_e$.

If we consider the dipole matrix elements both to the discrete state and the continuum, we can see interference effects between the discrete state, which alone would give rise to a resonance, and the hole induced in the continuum; this leads to the typical asymmetric line shape and possibly to antiresonances. Following the literature on the Fano effect, let us define

$$q=\frac{\tilde{T}_e}{\tilde{T}_0}\frac{V^*}{V}\ ;$$

then the expression (16) for the absorption assumes the form

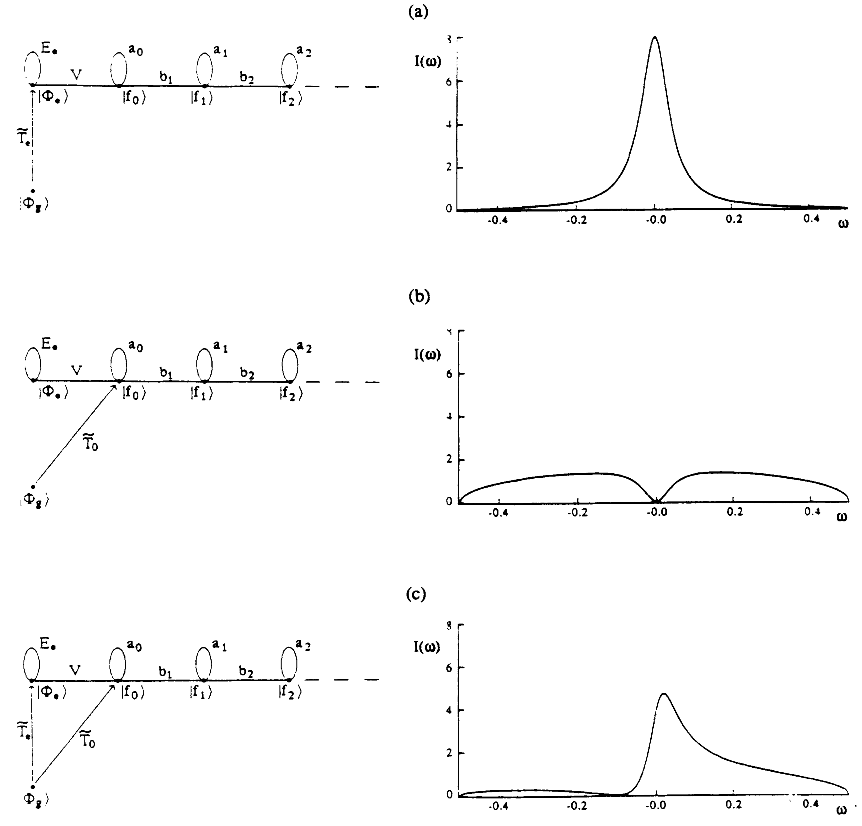

FIG. 3. Absorption line shape in the case of a discrete state interacting with a continuum described by a semielliptical density of states in the energy interval $(-W, W)$. The interaction $V$ equals one tenth of the band width. In (a) only the discrete state is dipole allowed. In (b) only the interaction carrying state is dipole allowed. In (c) both the discrete and the interaction carrying states are dipole allowed, and the asymmetry parameter $q$ is taken equal to 1.

$$n_\chi(E)=|\tilde{T}_0|^2\frac{|E+q|V||^2}{E^2+\Delta^2}\left[\frac{2}{\pi W^2}\sqrt{W^2-E^2}\right] . \qquad (18c)$$

We can easily recognize the two previous cases (18a) and (18b) as particular cases of (18c). When $q$ is real (and positive) the line shape (18c) is shown in Fig. 3(c); due to the fact that $q$ is real, the absorption vanishes at $E=-q|V|$. If, on the other hand, $q$ is a pure imaginary number, the interference term [due to the cross product in (18c)] is zero: no antiresonance appears, and we have only the sum of the two terms corresponding to the two transitions.

The results of the example discussed so far have been reported here to illustrate the convenience and simplicity of our procedure. Essentially equivalent effects would be obtained with rectangular density of states (10), whose self-energy is easily deducible from Eq. (11).

As a further illustrative example of our procedure, we consider the less studied although very interesting problem of the narrowing of the absorption spectrum arising in the case of two degenerate (or nearly degenerate) discrete states interacting with a continuum. Let us suppose for simplicity that the interaction matrix elements $V_{1i}$ and $V_{2i}$ are constant in the range $(-W, W)$ and negligible outside it; introducing the concept of the interaction carrying state we arrive at the Hamiltonian indicated schematically in Fig. 4. Treating the semi-infinite chain with the renormalization procedure we obtain an equivalent effective Hamiltonian in the space of the discrete states $|\Phi_1\rangle$, $|\Phi_2\rangle$ and the interaction carrying state $|f_0\rangle$:

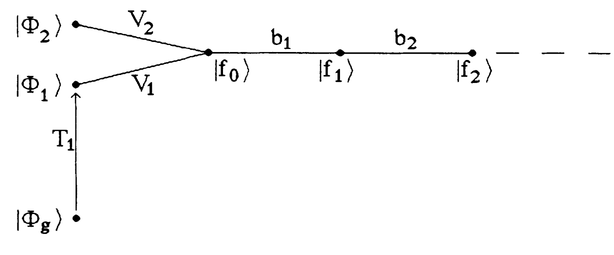

FIG. 4. Model Hamiltonian of a system with two degenerate states $(E_1=E_2)$ interacting with a continuum. The state $|\Phi_1\rangle$ is optically connected to the ground state.

$$
\begin{aligned}
H_{\mathrm{eff}}(E)=E_1|\Phi_1\rangle\langle\Phi_1|+E_2|\Phi_2\rangle\langle\Phi_2|+\sum(E)|f_0\rangle\langle f_0|\\
+(V_1|\Phi_1\rangle\langle f_0|+V_1^*|f_0\rangle\langle\Phi_1|)\\
+(V_2|\Phi_2\rangle\langle f_0|+V_2^*|f_0\rangle\langle\Phi_2|)\ ,
\end{aligned}
\tag{19}
$$

where $\sum(E)$ is the self-energy of the chain.

It is now simple to calculate the Green's function $G(E)=(E-H_{\mathrm{eff}})^{-1}$ in the space spanned by $|\Phi_1\rangle,|\Phi_2\rangle$ and $|f_0\rangle$; we find

$$
G(E)=\frac{1}{D(E)}\begin{vmatrix}
(E-E_2)\left[E-\sum(E)\right]-|V_2|^2 & V_1V_2^* & (E-E_2)V_1\\
V_1^*V_2 & (E-E_1)\left[E-\sum(E)\right]-|V_1|^2 & (E-E_1)V_2\\
(E-E_2)V_1^* & (E-E_1)V_2^* & (E-E_1)(E-E_2)
\end{vmatrix}\ ,
\tag{20}
$$

where we have indicated

$$
\begin{aligned}
D(E)=(E-E_1)(E-E_2)\left[E-\sum(E)\right]\\
-(E-E_1)|V_2|^2-(E-E_2)|V_1|^2\ .
\end{aligned}
$$

In the general case of dipole-allowed transitions to the states $|\Phi_1\rangle,|\Phi_2\rangle,|f_0\rangle$, with normalized matrix elements $\tilde{T}_1,\tilde{T}_2,\tilde{T}_0$, respectively, the dipole carrying state is

$$
|\chi\rangle=\tilde{T}_1|\Phi_1\rangle+\tilde{T}_2|\Phi_2\rangle+\tilde{T}_0|f_0\rangle\ .
$$

The Green's-function matrix element $G_{\chi\chi}(E)$ can be calculated and from it the absorption line shape deduced; $G_{\chi\chi}(E)$ contains the terms due to the transitions from the ground state to the discrete states and to the continuum, and those due to the interference between them.

To make even more transparent the analytic structure of the various contributions, and the related physical effects, consider the case in which the continuum is dipole forbidden, the two discrete states are degenerate ($E_1=E_2$), and an appropriate combination of them (relabeled, say, $|\Phi_1\rangle$) is dipole allowed as shown in Fig. 4.

The absorption line shape is determined by the imaginary part of $G_{11}(E)$, with

$$
G_{11}(E)=\frac{(E-E_1)\left[E-\sum(E)\right]-|V_2|^2}{(E-E_1)^2\left[E-\sum(E)\right]-(E-E_1)(|V_2|^2+|V_1|^2)}\ .
$$

By simple algebraic transformation, the above expression becomes

$$
G_{11}(E)=\frac{|V_2|^2}{|V_1|^2+|V_2|^2}\,\frac{1}{E-E_1}+\frac{|V_1|^2}{|V_1|^2+|V_2|^2}\,\frac{1}{(E-E_1)-\dfrac{|V_2|^2+|V_1|^2}{E-\sum(E)}}\ ,
\tag{21}
$$

and we recognize that the absorption spectrum is made by a δ function at $E_1$ superimposed to the spectrum that would occur in the absence of the state $|\Phi_2\rangle$, and an effective interaction $\sqrt{|V_1|^2+|V_2|^2}$ between $|\Phi_1\rangle$ and $|f_0\rangle$.

It is of interest to comment on the arising of the line narrowing in δ-like shape embodied in Eq. (21). The qualitative mechanism for its appearance is as follows. The effect of the discrete state $|\Phi_2\rangle$ on the continuum density of states is the depletion indicated in Fig. 3(b): a hole is carved in the density of states at the energy corresponding to the discrete state. In our case a second discrete state $|\Phi_1\rangle$ dipole connected to the ground state and degenerate with $|\Phi_2\rangle$ exists. Thus the autoionization of the discrete state $|\Phi_1\rangle$ is now, at least partially, quenched and a δ-like contribution remains unmasked. This argument is supported by the fact that if the two discrete states are not degenerate, the δ-like contribution converts into a sharp resonance and then into a standard resonance when the difference $E_2-E_1$ increases.

We can also understand the reasons of the intensities $B_1=|V_1|^2/(|V_1|^2+|V_2|^2)$ and $B_2=|V_2|^2/(|V_1|^2+|V_2|^2)$ of the two components of the spectrum of Eq. (21). A discrete state of energy $E_1$ interacts with states in the approximate interval $E_1\pm\Delta_1$, with $\Delta_1=2|V_1|^2/W$ [Eq. (17)] as we have seen in Fig. 3(a). At the same time the halfwidth of the spectral hole due to the state $|\Phi_2\rangle$ is $\approx\Delta_2$, with $\Delta_2=2|V_2|^2/W$; so if $|V_1|\ll|V_2|$ we understand why in the absorption line shape the δ-like contribution is prevalent with respect to the broad part of the spectrum. On the other hand, for $|V_1|\gg|V_2|$ the state $|\Phi_1\rangle$ does not feel the hole, and the spectrum is not influenced by the presence of the state $|\Phi_2\rangle$.

Before concluding, it is of interest to remark on the resemblance between our model and the interference narrowing due to overlapping resonances in semiconductor quantum-well structures proposed in a paper of Maschke, Thomas, and Göbel;[13] in their model[13] there are two interacting continua and one of them is optically active in a very small energy region and appropriately discretized.

## IV. CONCLUSIONS

In this paper we have revisited the long-standing problem of the absorption line shape of discrete states interacting with one or more continua of states; the problem is handled with the iterative techniques based on the recursion and the renormalization methods. Basically the continuum of states is mapped rigorously into one or more linear chains; the introduction of the concepts of the interaction and dipole carrying states allows to develop a formalism which is at the same time manageable and elegant. We have examined several illustrative examples, of absorption line shapes with significative occurrence of resonances, antiresonances, and line narrowing. The flexibility and generality of our formalism should be of value in all the problems concerning configuration mixing of electronic, excitonic, and vibrational spectra of solids.

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