

## Analysis of coalescent resonances in atom-surface scattering

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A special type of atom-surface resonance is analyzed, called coalescent resonances, which display an unusual broadening effect in their width. It is shown that the Fermi golden rule does not apply for these resonances.

### I. INTRODUCTION

Resonances are one of the most interesting phenomena in inelastic collisions. They have been studied in various systems and their theory is by now very well established. Basically, formation of a resonance is noticed as a rapid change of the cross section in a small vicinity of certain collision energy. The structure of this change carries information about the properties of resonance and in particular the width of this change is related to the lifetime of resonance.<sup>1</sup> This relationship is basic to all resonance phenomena and its universality has been recognized in many different areas of physics (e.g., lifetime of many elementary particles is determined in this way).

The width of inelastic resonances is also related to the value of coupling between the channels and therefore from the observed cross section it is possible to obtain some information about the system. This relationship tells us that if a system has one or more bound states in closed channels, when coupling between channels is neglected, then these bound states will appear as resonances (of Feshbach type<sup>2</sup>) when coupling with open channels is introduced. In fact, it was shown that the width of these resonances is proportional to the second order in the coupling strength.<sup>3</sup> This rule is so general that it acquired the name the Fermi golden rule.<sup>4</sup> For example, on the basis of this rule (but *not only* because of it) weak interactions in high energy physics were selected as a separate force in nature.<sup>5</sup> Pictorially what the rule says is that a resonance can only be formed if the system makes a transition from one open channel into the closed one and back into an open channel.<sup>6</sup> Therefore, formation of a resonance is a two-stage process, which is reflected in the relationship between the width of the resonance and the magnitude of coupling between the channels.

That this rule may not always hold true will be shown here. We will show this with the example of special resonances which are formed in atom-surface scattering. However, this example is not the only one. Analogous circumstances are, for example, met when the electromagnetic waves are scattered on a planar array of metal spheres, arranged in a regular pattern (for instance, rectangles) and immersed in a dielectric medium. The dielectric medium has a certain thickness above the plane and plays the role of an attractive atom-surface potential. Another circumstance in which this rule does not hold

true is the case of elastic collisions of two particles, when zero-angular-momentum resonances are formed.<sup>7,8</sup>

As we have said, we will describe these resonances with the example of atom-surface collisions.<sup>9</sup> However, because of the specific nature of atom-surface collisions, we will briefly outline the main points of the theory. Typical of atom-surface collisions is that atoms are scattered on a potential which is periodic in the surface plane. Therefore, if the  $z$  axis is perpendicular to the surface, the potential can be written in the form of expansion

$$V(x,y,z) = \sum_{m,n} e^{iG_m x + iG_n y} V_{m,n}(z), \quad (1.1)$$

where  $\vec{G}_m$  and  $\vec{G}_n$  are the inverse lattice vectors, defined by

$$G_m = \frac{2\pi}{a} m, \quad G_n = \frac{2\pi}{b} n, \quad (1.2)$$

where  $a$  and  $b$  are the lattice constants. The form of (1.1) implies that the scattering wave function is also periodic in the  $x$  and  $y$  direction and that it has the expansion

$$\psi(x,y,z) = e^{ik_x x + ik_y y} \sum_{m,n} \varphi_{m,n}(z) e^{iG_m x + iG_n y}, \quad (1.3)$$

where  $k_x$  and  $k_y$  are projections of the initial wave number (momentum) of the atom on the  $x$  and  $y$  axes, respectively.

The Schrödinger equation for the atom-surface system is

$$[T + V(x,y,z)]\psi = E\psi,$$

where  $T$  is the kinetic energy of the atom. When  $\psi$  is replaced by expansion (1.3) we obtain a set of equations for  $\varphi_{m,n}$  which has the form

$$\begin{aligned} \varphi_{m,n}'' &= -[k^2 - (k_x + G_m)^2 - (k_y + G_n)^2] \varphi_{m,n} \\ &+ \sum_{m',n'} V_{m-m',n-n'}(Z) \varphi_{m',n'}. \end{aligned} \quad (1.4)$$

The set of equations (1.4) when solved for the following boundary condition at  $z \rightarrow \infty$ ,

$$\varphi_{m,n}(Z) \sim e^{-ik_z^{(m,n)} z} + \sum_{m',n'} e^{ik_z^{(m',n')} z} S_{m,m';n,n'}, \quad (1.5)$$

describe the scattering of the atoms on the surface. The values  $|S_{m,m';n,n'}|^2$  give transition probabilities from the

channel  $(m, n)$  into the channel  $(m', n')$ . The  $Z$  component of the wave number (momentum) is

$$(k_z^{m,n})^2 = k^2 - (k_x + G_m)^2 - (k_y - G_n)^2, \quad (1.6)$$

where  $k$  is the initial wave number (momentum). For simplicity we will from now on omit the indices  $(m, n)$  of  $k_z$ .

The structure of Eqs. (1.4), together with the boundary condition (1.5), is very similar to the multichannel equations appearing in many other problems such as electron-atom, atom-atom, atom-molecule, nuclear, and even high-energy collisions. However, the meaning of channels is slightly different in atom-surface collisions; here the two indices of a channel are associated with different diffraction peaks, while usually different channels are associated with different states of a system (e.g., electronic states of molecules, different particles, etc.). Conceptually there is no difference, except that in the atom-surface collisions one should take care when trying to interpret cross sections; they have meaning for the intensity of diffraction peaks and not the intensity of scattered particles in different directions.

The position of diffraction peaks is easily obtained by evaluating the current of particles

$$\vec{j} \sim \text{Im}(\psi^* \vec{\nabla} \psi), \quad (1.7)$$

where  $\psi$  is (1.3) and  $\psi_{m,n}$  are asymptotically given by (1.5). We obtain for the current of outgoing particles in the channel  $(m, n)$

$$\vec{j}_{m,n} \sim (k_x + G_m)\hat{x} + (k_y + G_n)\hat{y} + k_z\hat{z}, \quad (1.8)$$

where  $\hat{x}$ ,  $\hat{y}$ , and  $\hat{z}$  are unit vectors along appropriate axes. It means that  $G_m$  and  $G_n$  represent components of a pseudomomentum in the  $x$ - $y$  plane, which scatter the initial momentum  $\vec{k}$  into another direction, while at the same time preserving its modulus [ $k_z$  is calculated from (1.6) so that this is always true]. This is a pictorial way in which we can obtain the position of the diffraction peaks using vectors. In the special case when  $m = n = 0$  the diffraction peak is at the position where atoms are scattered by simple reflection, as on a mirror. Because of its unique position, this peak is also named specular. All other peaks are obtained with respect to the specular, by evaluating the vector (1.8).

One can show that only a finite number of diffraction peaks are observed, but an infinite number of them give imaginary values for  $k_z$ , therefore they are not observed. The meaning of these channels is the same as in the other multichannel scattering; they represent closed channels and are only meaningful when atom-surface potential has attraction. In such a case the atom may form a bound state in a closed channel if its energy coincides with the energy of one of the bound states of the potential. Of course such a bound state will not have infinite lifetime, because the atom has the possibility to "get out" into an open channel. As a result we will observe a rapid change of intensity of diffraction peaks in the neighborhood of the collision energy when in one closed channel such a bound state is formed. Since the bound states of potential are discrete, it is obvious that resonances are observed for

discrete values of collision energy.

Let us, for simplicity, restrict our discussion to resonances in the specular peak. As we have mentioned, a resonance will be observed in the specular peak  $\vec{k}_s = (k_{x_0}, k_{y_0}, k_{z_0})$ , if the initial momentum  $\vec{k}_0 = (k_{x_0}, k_{y_0}, -k_{z_0})$  is deflected by  $\vec{G}_0 = (G_{m_0}, G_{n_0})$  into the channel (or diffraction peak)

$$\vec{k} = (k_{x_0} + G_{m_0})\hat{x} + (k_{y_0} + G_{n_0})\hat{y} + k_z\hat{z} \quad (1.9)$$

and subsequently deflected into the specular peak. In the channel (1.9)  $k_z$  is imaginary, therefore  $\vec{k}$  does not have the meaning of the position of the real diffraction peak. We have written  $\vec{k}$  in the form (1.9) so that we will better understand the properties of coalescent resonances.  $k_z$  for a resonance should be equal to

$$k_z^2 = -k_b^2, \quad (1.10)$$

where  $-k_b^2$  is the energy (in units of wave-number squared) of bound states of the atom-surface potential  $V_{0,0}$  [see Eq. (1.4)].

From Eq. (1.10) we obtain the values of  $k_{x_0}$  and  $k_{y_0}$  for which the resonance is observed in the specular peak. It is obvious from the definition of  $k_z^2$  in (1.6) that there is no unique solution of (1.10), and that there is a whole range of values of initial  $k_{x_0}$  and  $k_{y_0}$  for which the same resonance is observed [we will talk about the "same resonance" when for a class of resonances the condition (1.10) is satisfied for a given  $\vec{G}_0$ ]. Therefore, one component of  $\vec{k}$  in the  $x$ - $y$  plane should be arbitrarily chosen (for instance,  $k_{y_0}$ ), while the other ( $k_{x_0}$ ) is obtained from (1.10) and (1.6). We obtain two solutions

$$k_{x_0} = -G_{m_0} \pm [k^2 + k_b^2 - (k_{y_0} + G_{n_0})^2]^{1/2}, \quad (1.11)$$

which means that there are two values of  $k_{x_0}$  (for the given values of  $k^2$  and  $k_{y_0}$ ) for which the atom can be trapped in the bound state of energy  $-k_b^2$ , when it is scattered by momentum  $\vec{G}_0$  [of course, if the square root in (1.11) is real]. Therefore, the same resonance appears in the specular peak for two values of  $k_{x_0}$ , when  $k_{y_0}$  is chosen arbitrarily; the coordinates of one specular peak are  $(k_{x_0}^+, k_{y_0}, k_z^+)$  and of the other  $(k_{x_0}^-, k_{y_0}, k_z^-)$ , where  $k_{x_0}^\pm$  refers to one of the values in (1.11) and

$$k_z^\pm = [k^2 - k_{y_0}^2 - (k_{x_0}^\pm)^2]^{1/2}. \quad (1.12)$$

If one (or all) of the values in (1.12) are imaginary, then the corresponding specular peak is nonphysical and only one (or none) will be observed. In what follows we will assume that both specular peaks are physical.

Let us now assume that for a given  $k_{y_0}$  we scan  $k_{x_0}$  [ $k_z$  for the specular peak is then uniquely determined from (1.6), when  $\vec{G}_0 = \vec{0}$ ] and follow the specular peak by measuring its intensity. Then at the two positions, given by (1.11), we will observe a resonance, which is formed in the channel  $\vec{G}_0$ . In fact we observe the same resonance which appears at two different locations. When we now

take a different value for  $k_{y_0}$  it is obvious that the location of the two resonance peaks will be different. However, there is a particular value of  $k_{y_0}$  for which these two resonance peaks will merge and this is when in (1.11) we have

$$k^2 + k_b^2 - (k_{y_0} + G_{n_0})^2 = 0.$$

In such a case we talk about the coalescence of two resonances and this effect will be studied in this paper. As will be shown, the properties of coalescent resonances cannot be easily explained in terms of the classical resonance theory. We will also show that the Fermi golden rule does not apply for them.

In all our discussions we have implicitly assumed that coupling between channels is weak, in which case location of resonances is determined from Eq. (1.10). In the rest of this paper we will therefore use the perturbation theory. However, it is believed that the properties of these resonances are the same when coupling is strong, but then one should use a different scheme for their study.

In the preceding discussion we have used the Cartesian coordinates for momentum  $\vec{k}$  because of their simplicity. In practice, it is more convenient to use the polar coordinates  $k$ ,  $\theta$ , and  $\phi$ , where  $k$  is the modulus,  $\theta$  is the polar angle, and  $\phi$  is the azimuthal angle of  $\vec{k}$ . In such a case the channel energy (1.6) becomes

$$k_z^2 = k^2 \cos^2 \theta - G^2 - 2kG \sin \theta \cos(\phi - \phi_G) \equiv K_G^2, \quad (1.13)$$

where

$$G = (G_m^2 + G_n^2)^{1/2}, \quad \phi_G = \tan^{-1}(G_n/G_m). \quad (1.14)$$

Equation (1.10) now has a solution in one of three variables  $k$ ,  $\theta$ , or  $\phi$ , but in our discussion we will assume that  $\theta$  and  $\phi$  are given and  $k$  is calculated. In such a case we find two solutions for  $k$ ,

$$k_{1,2} = \frac{k_0 \pm [k_0^2 - (k_b^2 - G_0^2) \cos^2 \theta]^{1/2}}{\cos^2 \theta} \quad (1.15)$$

where

$$k_0 = G_0 \sin \theta \cos(\phi - \phi_G). \quad (1.16)$$

The meaning of two solutions for  $k$  is that for a given position of specular peak, determined by  $\theta$  and  $\phi$ , the same resonance in the channel  $\vec{G}_0$  is observed for two values of  $k$  (or energy) if both  $k_{1,2}$  are positive. However, when in (1.15) the square root is zero, the two resonance peaks merge into a single one, which happens when

$$\begin{aligned} \cos \theta_c &= \frac{1}{k_0} (k_b^2 - G_0^2)^{1/2}, \\ \cos(\phi_c - \phi_G) &= \left[ \frac{k_b^2}{G_0^2} - 1 \right]^{1/2} \cot(\theta_c), \end{aligned} \quad (1.17)$$

where  $k_0$  has arbitrary value, which depends on our choice of initial energy for which we want to observe the coalescence of two resonances.

## II. PERTURBATION THEORY OF COALESCENT RESONANCES

In order to understand the nature of coalescent resonances we will use the perturbation theory. It has already been used in the zeroth order in the Introduction in order to explain the source of such resonances, but their properties can only be derived when coupling between channels is introduced. There are several approximate perturbation schemes which can be used for this purpose, but we will use the one which has been developed as a general perturbation theory of resonances.<sup>10</sup>

It is very convenient to represent a resonance by a complex pole in  $k$  of the  $S$  matrix (it should be recalled that  $k$  was defined in the Introduction, and was assumed to be an independent variable). This pole is also a root of the equation<sup>11</sup>,

$$F(k) = \det[J(k)] = 0, \quad (2.1)$$

where  $J$  is the Jost function (in fact a matrix, but for convenience we will refer to it as a function) for the set of coupled equations (1.4). If we replace the off-diagonal elements of  $V_{\vec{G}-\vec{G}'}$  by  $\epsilon V_{\vec{G}-\vec{G}'}$ , where  $0 \leq \epsilon \leq 1$ , then (2.1) is also a function of  $\epsilon$ . Therefore a root of (2.1) will also be a function of  $\epsilon$ , so in general we can write

$$k_p^{(G)} = k_0^{(G)} + \epsilon k_1^{(G)} + \frac{\epsilon^2}{2} k_2^{(G)} + \dots, \quad (2.2)$$

where  $k_p^{(G)}$  is the root of (2.1). In the limit  $\epsilon \rightarrow 0$  its value is given by (1.15).

The coefficients in (2.2) can be calculated in a closed form,<sup>10</sup> but this procedure, in the case of the coalescent resonances, cannot be applied for the reason which will become apparent later. Instead we must slightly modify the set of equations (1.4). We first calculate  $k$  from (1.13) when we obtain

$$k_{1,2} = \frac{k_0 \pm [k_0^2 + (k_G^2 + G^2) \cos^2 \theta]^{1/2}}{\cos^2 \theta}, \quad (2.3)$$

where  $k_0 = G \sin \theta \cos(\phi - \phi_G)$ . Although  $k$  is not unique, we can choose one of the values in (2.3) and replace  $k$  in all other channels in (1.4). The set of coupled equations now becomes a function of  $K_G$  and the controlling parameters (by the controlling parameters we mean the variables  $\theta$  and  $\phi$ , which are fixed when  $k$  is scanned). Because of this change we no longer look for the roots of  $F$  in  $k$  but in the variable  $K_{\vec{G}}$ . Hence (2.1) is

$$F(K_{\vec{G}}; \epsilon) = 0 \quad (2.4)$$

and the expansion (2.2) becomes

$$K_{\vec{G}}^{(p)} = K_{\vec{G}}^{(0)} + \epsilon K_{\vec{G}}^{(1)} + \frac{\epsilon^2}{2} K_{\vec{G}}^{(2)} + \dots \quad (2.5)$$

As it has been shown,<sup>10</sup> if the perturbation  $\epsilon V_{\vec{G}-\vec{G}'}$  is an off-diagonal matrix, and  $K_{\vec{G}}^{(0)}$  is not degenerate (i.e., there is no other  $\vec{G}'$ , for which  $K_{\vec{G}}^{(0)} = K_{\vec{G}'}^{(0)}$ ), then

$$K_G^{(1)} = 0. \quad (2.6)$$

Hence to the second order in  $\epsilon$

$$K_G^{(p)} = K_G^{(0)} + \frac{\epsilon^2}{2} K_G^{(2)}, \quad (2.7)$$

where  $K_G^{(2)}$  is complex.

However, in the vicinity of a resonance, the  $S$  matrix is parametrized as

$$S \sim \frac{\beta}{k - k_p^{(G)}} + b, \quad (2.8)$$

where  $\beta$  is the matrix of residues and  $b$  is the matrix for background scattering. Therefore the variable  $K_G^{(p)}$ , for which we have found expansion coefficients in (2.7), does not enter explicitly the parametrization of the  $S$  matrix, but the variable  $k_p^{(G)}$ , for which these coefficients have to be found. These coefficients are found by calculating the channel energy  $K_G^2$  in (1.13). For  $K_G$  we take expansion (2.7) and for  $k$  we take expansion (2.2) and compare the coefficients of the like powers in  $\epsilon$ . For example, the coefficients with the power  $\epsilon^0$  give

$$k_0^{(G)} = k_{1,2}, \quad (2.9)$$

where  $k_{1,2}$  are given by (1.15), if we assume that  $K_G^{(0)} = ik_b$ . Comparison of coefficients of the order  $\epsilon$  gives

$$0 = k_1^{(G)} [2k_{1,2} \cos^2 \theta - 2G \sin \theta \cos(\phi - \phi_G)], \quad (2.10)$$

where  $k_{1,2}$  designates one of the values from (1.15). It follows from (2.10) that

$$k_1^{(G)} = 0 \quad (2.11)$$

if the term in the bracket is nonzero. The bracket is zero for

$$k_1 = \frac{G \sin \theta \cos(\phi - \phi_G)}{\cos^2 \theta} \quad (2.12)$$

and this is just the value of  $k_1$  and  $k_2$ , when two resonance peaks merge into one [see Eq. (1.15)]. Therefore, for two resonance peaks, when they are not close, the first-order perturbation coefficient in (2.2) is identically zero. But when two resonance peaks merge into a single one, this coefficient is nonzero. Its value, for such a case, can be obtained by comparing the coefficients in (1.13) of the second order in  $\epsilon$ . We get

$$2ik_b K_G^{(2)} = 2(k_1^{(G)})^2 \cos^2 \theta + 2k_2^{(G)} [k_{1,2} \cos^2 \theta - G \sin \theta \cos(\phi - \phi_G)] \quad (2.13)$$

and for merged resonances the last term in (2.13) is zero. Therefore

$$ik_b K_G^{(2)} = (k_1^{(G)})^2 \cos^2 \theta \quad (2.14)$$

from which we find the explicit value of the coefficient  $k_1^{(G)}$  in (2.2). When two resonance peaks are well separated then the second-order coefficient  $k_2^{(G)}$  is

$$k_2^{(G)} = \frac{ik_b K_G^{(2)}}{k_{1,2} \cos^2 \theta - G \sin \theta \cos(\phi - \phi_G)}, \quad (2.15)$$

in which case the perturbation series (2.2) is similar in structure to the series (2.7), i.e., the second-order term in  $\epsilon$  is the leading correction in the perturbation series.

Using these formulas we can now analyze in what way the coalescent resonances are different from the other type of resonances. When two resonance peaks are well separated, their positions are approximately given by

$$k_p^{(G)} \sim k_0^{(G)} + \frac{1}{2} k_2^{(G)}, \quad (2.16)$$

where  $k_0^{(G)}$  and  $k_2^{(G)}$  are given by (2.9) and (2.15), respectively. Since the width and the resonance shift are contained in the second term in (2.16), they are of the second order in  $\epsilon$ . Therefore, in this respect there is no difference between these and other types of resonances. However, it should be recalled that  $k_0^{(G)}$  and  $k_2^{(G)}$  have two values, depending on whether we choose the plus or minus sign in (1.15) [see Eqs. (2.9) and (2.15)] and these two values correspond to two resonance peaks. If we take the plus sign in (1.15), i.e., we take  $k_0^{(G)} = k_1$  in (2.16), then the appropriate resonance is described by the pole in the lower half of the  $k$  plane. This follows from the fact that  $\text{Re}(K_G^{(2)})$  is negative<sup>10</sup> and that the denominator in (2.15) must be positive [see Eq. (1.15) and the discussion which follows]. On the other hand, if we take the minus sign in (1.15) [ $k_0^{(G)} = k_2$  in (2.16)], then the denominator in (2.15) is negative and the appropriate pole of this resonance is in the upper half of the  $k$  plane. In this respect, properties of these resonances are different from ordinary resonances, which are described by the poles from only one half of the  $k$  plane (lower half).<sup>12</sup>

The value of  $k_0^{(G)}$  and  $k_2^{(G)}$  in (2.16) is a function of the controlling parameters, defined earlier. Therefore, when these parameters are varied, the two peaks move in two different parts of the complex  $k$  plane; one in the lower half and the other in the upper half. However, depending on whether  $k_{1,2}$  in (1.15) are real or complex, we distinguish two domains of the controlling parameters: in one, the two values  $k_{1,2}$  are real and in the other, they are complex. In the first domain and when two resonances are well separated, the movement of the appropriate poles is accurately described by (2.16). In the second domain, when the magnitude of the imaginary parts of  $k_{1,2}$  is large, the position of the poles is also very well described by (2.16). However, in the transition region, when  $k_1 \sim k_2$ , we cannot use the estimate (2.16) and instead the position of the poles is given by

$$k_p^{(G)} \sim k_0^{(G)} + k_1^{(G)}, \quad (2.17)$$

where  $k_1^{(G)}$  is given by (2.14). In this way we can follow the movement of poles in the whole range of definition of the controlling parameters.

The pictorial meaning of Eqs. (2.16) and (2.17) is the following. When the controlling parameters are in the domain when  $k_1$  and  $k_2$  are real, movement of the poles is on the opposite sides of the real  $\vec{k}$  axis. As the controlling parameters make transitions from one domain into the other, the two poles "collide," repel each other, and go into the complex  $k$  plane in opposite directions. After "collision" one pole is approximately the complex conjugate of the other pole.

From such behavior of the poles we can make a qualitative assessment of how the resonances will be observed in diffraction peaks. When  $k_{1,2}$  are real and well separated,

then resonances will be observed separately. As the controlling parameters approach the transition region of their two domains, the width of resonances will get wider according to the estimate (2.17), until the point when two resonances merge together. They only seemingly merge together because, as we have mentioned earlier, their corresponding poles are well separated in the complex  $k$  plane. But, because the real parts of these poles is nearly the same, the two resonances will be noticed as a single, very broad resonance. The width of this resonance is much larger than the width of the separated resonances and in order to give it a name we will call it a "giant resonance." It is exactly the width of the giant resonance which distinguishes the coalescent resonances from the other type of resonances. This point we will discuss in more detail after we give a few examples of coalescent resonances.

### III. EXAMPLES

We will demonstrate here the effect of coalescent resonances on the intensity of diffraction peaks. We will show this on the model calculation with five channels (0,0), (1,0), (0,1), (-1,0), and (0,-1). For diagonal elements of the potential matrix we take

$$V_{\vec{0}} = \begin{cases} -19.28 \text{ \AA}^{-2}, & Z \leq 2 \text{ \AA} = Z_1 \\ 0, & Z > Z_1 \end{cases} \quad (3.1)$$

while all coupling matrix elements are nonzero and equal to

$$V' = \begin{cases} 1 \text{ \AA}^{-2}, & Z \leq Z_1 \\ 0, & Z > Z_1 \end{cases} \quad (3.2)$$

except the elements which couple channels (1,0), (-1,0) and (0,1), (0,-1), which are zero. The potential  $V_{\vec{0}}$  supports three bound states,  $k_1^2 = -2.4077$ ,  $k_2^2 = -11.4602$ , and  $k_3^2 = -17.2986 \text{ \AA}^{-2}$ . For the lattice constant we have taken  $a = 2.84 \text{ \AA}$ .

For such potential the set of coupled equations (1.4) can be solved in a closed form and the  $S$  matrix, for the specular intensity, is<sup>11</sup>

$$S_{\vec{0}, \vec{0}} = \frac{f(-K_{\vec{0}})}{f(K)} \quad (3.3)$$

where<sup>13</sup>

$$f(K) = e^{iZ_1 K_{\vec{0}}} \det[U_p \cot(Z_1 p) \tilde{U} - iK] \quad (3.4)$$

and

$$P = \tilde{U}(K^2 - V)U \quad (3.5)$$

$K^2$  is the diagonal matrix of channel energies,  $V$  is the potential matrix, and  $U$  is the matrix which diagonalizes  $K^2 - V$ . In the expression (3.3) the meaning of  $f(-K_0)$  is that the wave number  $K_0$  in  $f(K)$  is formally replaced by  $-K_0$ .

The easiest way to look for the coalescent resonances is by taking the same arbitrary value of  $k$ , which is equal to the position of the giant resonance, i.e.,  $k = k_1 = k_2$ , where  $k_{1,2}$  are given by (1.15). Then we check whether

for this value of  $k$  there is  $-k_b^2$  for which we can find the appropriate values for  $\theta_c$  and  $\phi_c$ , given by (1.17). If the equations (1.17) have solutions, then this will be the approximate position of the giant resonance in  $\theta$  and  $\phi$ . If the same equations do not have solutions for any  $-k_b^2$ , then we must take another value for  $k$ . In our particular example we have taken  $k = 6.5 \text{ \AA}^{-1}$ , in which case for the bound state (0,1;2) (Ref. 14) we find solutions of (1.17) to be

$$\theta_c = 66.784^\circ, \quad \phi_c = 60.212^\circ \quad (3.6)$$

The dependence of these poles and resonances on the controlling parameters has been shown separately<sup>15</sup> and here we will only summarize the essential results. Movement of the poles is very well predicted by our approximate method (Fig. 1 of Ref. 15). Their trajectories are indeed in different parts of the complex  $k^2$  plane and are of hyperbolic shape.

Behavior of the corresponding resonances in the specular peak is also well described by our qualitative arguments (Fig. 2 of Ref. 15), however, the giant resonance is formed for slightly larger values of  $\theta$  than predicted by (3.6). This is understandable since (3.6) was obtained from an approximate treatment of resonance position. Apart from this, we notice the increase in width of the coalescent resonances as they approach each other. At the moment when they form the giant resonance, they are much wider than when they were separated.

Such simple behavior of coalescent resonances is not always found. For example, when  $k = 7 \text{ \AA}^{-1}$  and

$$\theta_c = 59.793^\circ, \quad \phi_c = 22.06^\circ \quad (3.7)$$

in addition to the two poles which correspond to the coalescent resonances and have source in the bound state (0,1;3), in the vicinity there is a third pole which corresponds to the bound state (0,1;1). This pole is there by accident, but its presence has a very interesting effect on the coalescent resonances, described in Ref. 15. However, even in such a case one observes formation of the giant resonance, although for slightly different values of  $\theta$  than predicted (see Fig. 4 of Ref. 15).

### IV. DISCUSSION

We have shown properties of a special type of resonance which we called the "coalescent resonances." They are found in atom-surface collisions and they come in pairs. The major feature of these resonances is that their resonance energy depends on the controlling parameters, i.e., the polar angle  $\theta$  and the azimuthal angle  $\phi$  of the specular peak. For some specific value of these parameters they merge together, while at the same time their width increases. We showed that this merger is not real because the appropriate poles of the two resonances move in different parts of the complex  $k$  plane. However, the fact remains that their width in diffraction peaks changes and it is exactly this feature which makes the coalescent resonances different from the other type of resonances. In order to see this, let us recall some aspects of the inelastic resonance phenomena.

The set of multichannel equations (1.4) is a typical

representative of equations which describe inelastic collisions, e.g., nuclear,<sup>16</sup> atomic and molecular,<sup>17,18</sup> electron-atom,<sup>19</sup> etc., which we will call generally the "particle collisions." Such a unique way of describing different processes will be reflected, among other things, in the fact that many properties of resonances will be common for all these systems. However, in one respect atom-surface collisions are fundamentally different from any other type of collisions and this is in the structure of the channel energy (we disregard the fact that also the centrifugal term is missing). In the particle collisions the channel energy is given as a difference  $E_n = E - \epsilon_n$  between the collision energy  $E$  and the threshold energy  $\epsilon_n$  of a particular channel, while in atom-surface collisions the form of channel energy is more complicated. Therefore in particle collisions there are no controlling parameters, as in the case of atom-surface collision, because the channel thresholds  $\epsilon_n$  are fixed quantities.

The approximate position of resonances is obtained by first decoupling the channel interaction and making one of the channel energies equal to the energy of a bound state of the channel potential (in our discussion we treat only Feshbach-type resonances). Therefore in particle collisions  $E_{\text{res}} = -E_b + \epsilon_n$  is the resonance energy, where  $-E_b$  is the energy of the bound state  $b$  in channel  $n$ . The appropriate wave number of this resonance is  $k_{\text{res}} = \pm(-k_b^2 + \chi)^{1/2}$ . It is obvious that only the plus sign has meaning. Therefore in these cases we never observe the pair of resonances which correspond to the same bound state and in the same channel. In atom-surface collisions, as we have seen, this pair is observed as coalescent resonances. If coupling between channels is now included, then  $-k_b^2$  becomes complex [arguments for this are the same as in the derivation of (2.4) and (2.5)], where the complex part is of the order  $O(\epsilon^2)$  in coupling. Therefore, near a resonance the  $S$  matrix parametrizes as

$$S \sim \frac{\beta}{k^2 - k_{\text{res}}^2} + b$$

and its width is of the order  $O(\epsilon^2)$ , even when  $\chi_n = k_b$ .

The reason why this is the case for resonances in particle collisions is that the point of coalescence of these resonances coincide with the threshold (i.e.,  $k=0$ ) while for the coalescent resonances this point can be for some nonzero value of wave number. Therefore in collisions where channel energy is given by  $E - \epsilon_n$ , the broadening effect of resonance cross sections can never be observed and the width of resonances in particle collisions is always second order in  $\epsilon$ . This law is quite general and in its simplest form is known as the Fermi golden rule,<sup>4</sup> which has found very broad application, ranging from particle physics to atom spectroscopy.

The rule that the width of resonances is second order in coupling also applies to degenerate resonances, although, as it has been shown,<sup>10</sup> the perturbation coefficient of the order  $\epsilon$  is nonzero. However, this coefficient contributes only to the level shift and not the width, which is for degenerate resonances also second order in coupling.<sup>10</sup>

Therefore, the broadening effect of the coalescent resonances is something unique to them, although the same effect was found, to a certain degree, for the zero-angular-momentum (ZAM) resonances.<sup>7,8</sup> Broadening of the width implies shorter lifetime of the resonance; however, it is not *a priori* clear that this is really what happens for the coalescent resonances. Usually, shorter (or longer) lifetime means a change in the dynamical properties of the system, e.g., change in the coupling strength between the channels, but the broadening effect of the coalescent resonances is of a kinematic nature, i.e., it only depends on the value of the controlling parameters. Therefore, there is no reason why the lifetime of these resonances should be shorter. Of course, these are only qualitative and nonrigorous arguments and therefore a more thorough study of this effect is needed.

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<sup>1</sup>See, for example, T. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Englewood Cliffs, 1962).

<sup>2</sup>The name "Feshbach Resonances" has been introduced in connection with the formalism developed in H. Feshbach, *Ann. Phys. (N.Y.)* **5**, 357 (1958).

<sup>3</sup>This fact follows directly from the Feshbach formalism. In addition to Ref. 2, see also A. I. Baz, Y. B. Zeldovich, and A. M. Perelomov, *Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics* (Israeli Program for Scientific Translation, Jerusalem, 1969).

<sup>4</sup>E. Fermi, *Nuclear Physics* (University of Chicago, Chicago, 1950), p. 142.

<sup>5</sup>Qualitative discussion about this point in R. Omnes, *Introduction to Particle Physics* (Wiley-Interscience, London, 1970), Chap. 1.6.

<sup>6</sup>This process is elegantly described using the Feynmann diagrams. The scattering, which involves an intermediate state (for instance, resonance), is represented by at least two vertices and one line which connects them.

<sup>7</sup>S. Bosanac, *Phys. Rev. A* **28**, 1344 (1983).

<sup>8</sup>S. Bosanac (unpublished).

<sup>9</sup>For a review of atom-surface scattering see H. Hoinkes, *Rev. Mod. Phys.* **52**, 933 (1980).

<sup>10</sup>S. Bosanac, *J. Math. Phys.* **23**, 2131 (1982).

<sup>11</sup>S. Bosanac and D. Micha, *J. Chem. Phys.* **73**, 6169 (1980).

<sup>12</sup>R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

<sup>13</sup>L. Fonda and R. G. Newton, *Ann. Phys. (N.Y.)* **10**, 490 (1960).

<sup>14</sup>Notation for bound state is  $(m, n; b)$  where  $m, n$  are two Miller indices and  $b$  is the vibrational quantum number.

<sup>15</sup>S. D. Bosanac, *Phys. Rev. A* (to be published).

<sup>16</sup>C. Mahaux and H. A. Weidenmüller, *Shell-Model Approach to Nuclear Reactions* (North-Holland, Amsterdam, 1969).

<sup>17</sup>M. S. Child, *Molecular Collision Theory* (Academic, London, 1974).

<sup>18</sup>W. H. Miller, *Dynamics of Molecular Collisions* (Plenum, New York, 1976).

<sup>19</sup>P. G. Burke, *Lect. Theor. Phys.* **11C**, 1 (1969).