Compound state resonances in the collinear collision of an atom with a diatomic oscillator*

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Compound state resonance effects are reported in exact, numerical calculations of the collinear collision of a particle with a harmonic oscillator with a Morse interaction potential. They are shown to be due to the formation of a long-lived complex or quasibound state and are much more narrow than resonances reported previously for this type of system. The stable eigenvalues resulting from a variational calculation with a bound state basis set are found to be in excellent agreement with the resonance energies, and such a variational calculation is a good way of locating these resonances.

INTRODUCTION

Compound state resonances are resonance effects in the scattering of a projectile from a target which are due to the formation of a long-lived, projectile–target complex. Such resonances have been observed experimentally in processes such as nuclear particle scattering[1] and in electron–atom collisions,[2] and a number of theoretical treatments of such phenomena exist.[3,4] In addition, compound state resonances have been found in calculations of the scattering of a particle from a rigid rotor.[5–7]

In this work, compound state resonances in the collinear collision of a particle with a harmonic oscillator are studied. This relatively simple model is often used to study molecular vibrational energy transfer without the complications introduced by the possibility of rotation and other processes.[8]

There appear to be two types of resonances in collinear collisions. The first type, which has been studied previously,[9] has been seen only for square well interaction potentials. These resonances are due to the formation of standing waves in the region of the attractive well[9] and might well be called shape resonances[8] in analogy with the shape resonances of potential scattering. The second type of resonance in collinear collisions is the compound state resonance reported here. These are seen for Morse interaction potentials which do not exhibit shape resonances. These resonances are very much narrower than the shape resonances; that is, the resonance effect occurs over a very narrow range of incoming particle energy. Another difference is that the inelastic vibrational transition probability decreases drastically at a compound state resonance whereas it increases or peaks at a shape resonance in all cases which have been calculated.

A number of collinear collision calculations have been carried out in the past with attractive well interaction potentials which exhibit fluctuations in the transition probability[9–15] which are often called resonances. One such calculation[10] involving a deeper attractive well than considered in this work exhibits a sequence of dips in the inelastic transition probability. Possibly these are compound state resonances of the type investigated here.

One motivation for this work was the desire to provide exact, quantum mechanical results for resonances in a simple, well-defined model. These may be used to evaluate approximate methods, in particular the semiclassical treatment of multidimensional bound states and resonances recently proposed by Marcus.[16]

The next section contains the results of scattering calculations in which compound state resonance effects are seen and provides the physical interpretation. The last section is a discussion of various methods of locating these very narrow resonances.

SCATTERING CALCULATIONS

The Schrödinger equation for the collinear collision of a particle with a harmonic oscillator may be reduced by proper choice of units[9,17] to

$$[-m^{-1}\partial^2/\partial x^2 - \partial^2/\partial y^2 + y^2 + V(x-y) - E]\Psi(x,y) = 0. \tag{1}$$

Here m is a mass ratio,[9] x is the coordinate of the incoming particle, y is the displacement from equilibrium of the oscillator, $V(x-y)$ is the interaction potential, and E is the total energy of the system in units of the zero point energy of the oscillator. The interaction potential is here taken to be a Morse potential which has the form

$$V(r) = d\exp(-\alpha r) - 2d\exp(-\tfrac{1}{2}\alpha r). \tag{2}$$

Here d is the depth of the attractive well and α determines the "steepness" of the attractive and repulsive parts of the potential.

The boundary conditions for Eq. (1) when the

oscillator is initially in the state denoted by i are

$$\Psi_i(x,y)_{x\sim-\infty} 0,$$

$$\Psi_i(x,y)_{x\sim\infty} \phi_i(y)\exp(-ik_i x) + \sum_n \phi_n(y)\exp(ik_n x)(k_i/k_n)^{1/2} S_{ni}\ , \tag{3}$$

where $\phi_n(y)$ is the wavefunction for a free oscillator which satisfies

$$(-\partial^2/\partial y^2 + y^2 - 2n - 1)\phi_n(y) = 0 \tag{4}$$

and $k_n^2 = m(E - 2n - 1)$. The matrix of coefficients S_{ni} is often called the S matrix.[18] The probability that the oscillator in state i will undergo a transition to state n is given by

$$P_{ni} = |S_{ni}|^2. \tag{5}$$

In what follows, use will be made of the phase of the S matrix defined by

$$S_{ni} = P_{ni}^{1/2}\exp(i\eta_{ni}) \tag{6}$$

where η_{ni} is real and ranges from 0 to 2π.

A series of calculations of S_{ni} for a range of energies E were performed for a number of mass, well depth, and steepness parameters m, d, and α. The method of amplitude density functions[19] was used to compute a reactance or K matrix, which is analogous to the S matrix defined as in Eq. (3) but with the complex exponentials replaced by sines and cosines.[20] Thus, solving for the K matrix involves only real arithmetic. The S matrix was then recovered from the K matrix by a suitable transformation.[20]

The resonances reported here are characterized by an extremely rapid increase by 2π of the phase of the S matrix η_{ni} with energy E. This occurs in the vicinity of certain distinct energies which are usually called the resonance energies. At these resonance energies the inelastic transition probabilities dip sharply and then rise again to the off-resonance value.

The behavior of the phase of the S matrix and the transition probability at a typical resonance is shown in Fig. 1. The rapid rise in η_{ni} and the dip in P_{ni} is clearly seen on this greatly expanded energy scale. The resonance occurs at an energy of $E = 3.642630$, which is above the threshold for excitation of the $n = 1$ vibrational state at $E = 3$ but below the threshold for the $n = 2$ state at $E = 5$.

To compute the S matrix accurately close to the resonance energy, it was necessary to include several more channels in the close coupling scheme and to take many, closely spaced integration steps. In the calculation reported in Fig. 1, eight channels were included and 5700 integration steps taken at $E = 3.6426298$, for example, while at $E = 3.6426200$ only four channels and 500 steps were necessary to obtain comparable accuracy.

Even with this amount of computation, it was not possible to adequately resolve the resonance in the ground state elastic phase η_{00}. It is not known whether the numerical method is not capable of resolving this resonance or whether the resonance in η_{00} does not exist.

The usual physical interpretation of this type of resonance is as follows. At the resonance energy, the incident particle "sticks" to the target for an abnormally long time compared with the particles incident at neighboring energies. The resonance is thus an indication of the formation of a quasi-bound or compound state, which in this case is a three-particle complex with a long but finite lifetime.

The evidence for this interpretation in the present case is twofold. First of all, it may be shown[21] that the time by which the incident particle is delayed by the interaction with the target oscillator is proportional to $d\eta_{ni}/dE$. Thus if η_{ni} rapidly increases by 2π at the resonance energy and returns to its previous, slowly changing behavior, the incident particle has been trapped by the target with a lifetime proportional to the rate of increase of η_{ni} with E.

On the other hand, one may evaluate the integral

$$\int_{-\infty}^{r}\int_{-\infty}^{\infty} |\Psi_i(x,y)|^2\, dy\, dx,$$

where r is large enough so that the integration is

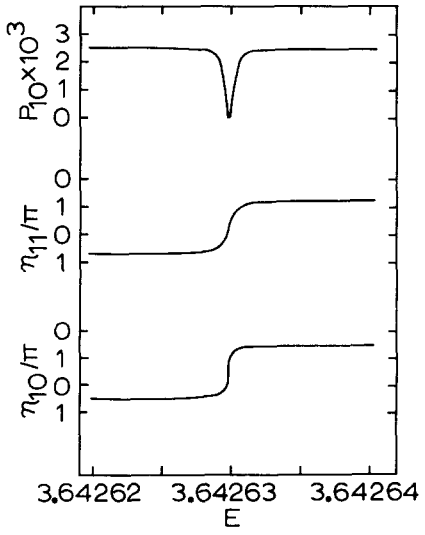

FIG. 1. The probability of a $1 \leftarrow 0$ vibrational transition and the phase of the S-matrix modulo 2π [cf. Eq. (6)] in the vicinity of a resonance. This collinear system has mass, steepness, and well depth parameters $m = 0.2$, $\alpha = 0.1$, $d = 1.5$, respectively.

over the whole region where the interaction potential is nonnegligible. This integral is a measure of the probability of finding the incident particle in the vicinity of the oscillator. In the Appendix it is shown that it is

$$\int_{-\infty}^{r}\int_{-\infty}^{\infty}|\Psi_i(x,y)|^2\,dy\,dx = r\left(1+\sum_n P_{ni}k_i/k_n\right)+\sqrt{P_{ii}}/k_i\,\sin(2k_i r+\eta_{ii}) + (2k_i/m)\sum_n P_{ni}(d\eta_{ni}/dE)\ . \quad (7)$$

It is clear from this result that close to a resonance energy where $d\eta_{ni}/dE$ is large, the last term will dominate and there will be a high probability of finding the incident particle in the vicinity of the target.

VARIATION AND PERTURBATION CALCULATIONS

It is very difficult to discover the location of the resonance energies by performing scattering calculations because the jump in the phase occurs over a very small range of energy. For example, to find all the resonances like the one in Fig. 1 between the thresholds for $1\leftarrow 0$ and $2\leftarrow 0$ vibrational transitions would require calculations at more than 4000 energies, which is a considerable computational effort. Better methods of locating the resonance energies, which have been found to be useful, will now be discussed.

From Eq. (7), one suspects that the amplitude of the wavefunction at a resonance energy will be large in the region where the potential is large. At nearby energies the amplitude will be much smaller. Thus the resonance wavefunction has the qualitative features of a bound state wavefunction. The difference is that, whereas a bound state wavefunction vanishes as the incoming particle coordinate approaches infinity, the resonance wavefunction oscillates in the manner given by Eq. (3). Thus it is reasonable to expect that a variational calculation of $\Psi(x,y)$ of Eq. (1) using a basis set of bound state wavefunctions will nearly converge to the resonance energy. This method of computing resonance energies was first proposed by Taylor[22,23] and was called the stabilization method. It was used successfully to compute resonances for simple models.[24-27]

In this work the scattering wavefunction was approximated by a set of harmonic oscillator eigenfunctions $\phi_n(y)$ defined by Eq. (4). That is, the wavefunction was written

$$\Psi(x,y)=\sum_{i,n} c_{in}\phi_i(\lambda x-\nu)\phi_n(y), \quad (8)$$

where λ and ν are adjustable parameters and the coefficients c_{in} are to be determined by the variational procedure. Substitution of Eq. (8) into Eq. (1) leads to the usual algebraic eigenvalue problem, which was solved by standard numerical methods.[28] This results in a large set of eigenvalues. The eigenvalues lying below energy $E=1$ are, of course, approximations to the true bound states of the three-body collinear system. Those lying above $E=1$ are not strictly eigenvalues of Eq. (1) and most of them do not converge to any limit as the size of the basis set is increased. However, a number of these higher eigenvalues do not change as the size of the basis set is increased. They are approximations to the resonance energies.

All of the computed eigenvalues which lie between $E=3.0$ and 4.5 are given in Table I for different basis sets. Although most of the eigenvalues are unstable, the underlined values do not change as the basis set is increased. It is seen that one of these stable eigenvalues is a good approximation to the resonance plotted in Fig. 1.

Table II gives resonance energies computed by a scattering calculation discussed in the last section compared to a variational calculation for various mass, depth, and steepness parameters m, d, and α. In most cases, of course, the variational calculation was performed first to locate the resonances, and the location was verified by a

TABLE I. Some higher eigenvalues of the collinear system.[a]

Size of basis set		
4×32[b]	4×36	4×40
3.0787	3.0559	3.0385
3.1870	3.1825	3.0810
3.2179	3.2647	3.1544
3.3746	3.3260	3.2865
3.4950	3.4848	3.3472
3.5477	3.5553	3.4334
3.6426[c]	3.6426	3.5942
3.7366	3.6585	3.6267
3.8041	3.8458	3.6426
3.8903	3.8561	3.7685
3.9408	3.8903	3.8903
4.1131	4.0484	3.9204
4.1451	4.1131	3.9560
4.1610	4.1851	4.1131
4.3110	4.2647	4.1560
4.3959	4.3110	4.2311
4.4840	4.4839	4.3110
	4.4940	4.3694
		4.4839

[a]Computed by diagonalizing the Hamiltonian matrix of Eq. (1) with $m=0.2$, $\alpha=0.1$, $d=1.5$ with the basis set given in Eq. (8) with $\lambda=0.15$, $\nu=2.0$.

[b]This notation means that 4 basis functions of y and 32 basis functions of x were used in Eq. (8).

[c]The underlined eigenvalues do not change with an increased basis set.

TABLE II. Resonance energies for various systems.

Scattering[a]	Variation[b]	First order[c]	Zero order[d]	Quantum No.[e]
	$m=0.2$	$\alpha=0.1$	$d=1.5$[f]	
1.63901	1.6390	1.6392	1.6338	0,1
1.887	1.8870	1.8875	1.8827	1,1
2.110	2.1101	2.1109	2.1065	2,1
2.308	2.3083	2.3092	2.3054	3,1
	2.4816	2.4826	2.4793	4,1
	2.6300	2.6309	2.6281	5,1
3.64263	3.6426	3.6428	3.6338	0,2
3.890	3.8903	3.8908	3.8827	1,2
4.113	4.1131	4.1138	4.1065	2,2
	4.3110	4.3118	4.3054	3,2
	4.4839	4.4848	4.4793	4,2
	4.6320	4.6328	4.6281	5,2
	$m=0.2$	$\alpha=0.1$	$d=3.0$	
2.209	2.209	2.2088	2.1905	0,2
	2.569	2.5699	2.5528	1,2
	2.904	2.9059	2.8901	2,2
3.215	3.214	3.2170	3.2024	3,2
3.500	3.500	3.5031	3.4897	4,2
3.761	3.761	3.7642	3.7520	5,2
3.998	3.997	4.0003	3.9893	6,2
4.218	4.218	4.2113	4.2016	7,2
	$m=0.5$	$\alpha=0.25$	$d=0.05$	
2.98239	2.9824	2.9824	2.9817	0,1
	4.9828	4.9829	4.9817	0,2

[a]Computed by a scattering calculation.
[b]Some of the stable higher eigenvalues from a variational calculation.
[c]Perturbation method including the first order correction.
[d]Zero order perturbation method.
[e]In the form n, i from Eqs. (11) and (16).
[f]These mass, steepness, and well depth parameters, respectively, are roughly appropriate for an inert atom–halogen molecule interaction.

scattering calculation. It is seen that the variational calculation accurately predicts the location of the resonances as expected.

In cases where there were many resonances, only the low-lying ones were computed here. The resonances lying close to the threshold for the next transition are difficult to approximate in the presence of lower resonances with the basis set used in Eq. (8). Also, these resonances are sharper than the low-lying ones and are even more difficult to find than the latter by means of a scattering calculation.

It turns out that, for the purpose of computing resonance energies, the incident particle and oscillator motions are nearly separable for most collinear systems of physical interest. Thus it is expected that perturbation methods would give a good approximation to the resonance energies.

For the purpose of using perturbation methods, the Hamiltonian in Eq. (1) is partitioned into a separable part and a perturbing potential as follows. The separable zero order Hamiltonian is

$$H^{(0)} = -m^{-1}\partial^2/\partial x^2 + V(x) - \partial^2/\partial y^2 + y^2, \tag{9}$$

where $V(x)$ is the Morse potential function defined in Eq. (2). The perturbation must be

$$H^{(1)} = V(x-y) - V(x). \tag{10}$$

The eigenvalues of $H^{(0)}$ are the sum of the harmonic oscillator eigenvalues given by Eq. (4) and the Morse oscillator eigenvalues[29] and are

$$E_{ni}^{(0)} = 2i + 1 - \alpha^2(a - n - \tfrac{1}{2})^2/(4m), \tag{11}$$

where

$$a = 2(md)^{1/2}/\alpha \tag{12}$$

and n is restricted to $0 \leq n < a - \frac{1}{2}$.

These zero order eigenvalues are compared in Table II with the numerically computed resonance energies. There is reasonable agreement in all cases in which variational and scattering calcula-

tions have been performed.

The first order shift in the eigenvalues due to the perturbation $H^{(1)}$ of Eq. (10) is given by the usual perturbation theory as

$$E_{ni}^{(1)} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \chi_n^*(x)\phi_i^*(y)[V(x-y)-V(x)] \times \chi_n(x)\phi_i(y)\,dx\,dy\ , \tag{13}$$

where $\phi_i(y)$ are harmonic oscillator wavefunctions defined by Eq. (4) and $\chi_n(x)$ are real, orthonormal eigenfunctions of the Morse oscillator Hamiltonian,[29]

$$-m^{-1}\partial^2/\partial x^2 + d\exp(-\alpha x) - 2d\exp(-\tfrac{1}{2}\alpha x). \tag{14}$$

Using the definition (2) for $V(x-y)$ and $V(x)$, Eq. (13) becomes

$$E_{ni}^{(1)} = d\int_{-\infty}^{\infty}\chi_n^2(x)e^{-\alpha x}dx\int_{-\infty}^{\infty}\phi_i^2(y)(e^{\alpha y}-1)\,dy - 2d\int_{-\infty}^{\infty}\chi_n^2(x)e^{-\alpha x/2}dx\int_{-\infty}^{\infty}\phi_i^2(y)(e^{\alpha y/2}-1)\,dy. \tag{15}$$

The integrals over the harmonic oscillator coordinate y are easily done[17] and those over the Morse oscillator coordinate x may be carried out by using a polynomial representation of the $\chi_n(x)$ eigenfunctions.[30] The result is

$$E_{ni}^{(1)} = (d/a)(a-n-\tfrac{1}{2})[K_i(\alpha)-2K_i(\alpha/2)], \tag{16}$$

where

$$K_i(\alpha) = \int_{-\infty}^{\infty}\phi_i^2(y)(e^{\alpha y}-1)\,dy = (2^i i!)^{-1}\exp(\alpha^2/4)\sum_{j=0}^{i}\binom{i}{j}^2 2^j j!\,\alpha^{2i-2j} - 1 \tag{17}$$

and a is given by Eq. (12).

The resonance energy correct to first order is given by the sum $E_{ni}^{(0)} + E_{ni}^{(1)}$ and appears in Table II. It is seen that the first order eigenvalue is in quite good agreement with the numerically computed resonance locations, much more so than the zero order eigenvalue.

APPENDIX

It is desired to evaluate the integral,

$$I = \int_{-\infty}^{r}\int_{-\infty}^{\infty}\Psi_i^*(x,y)\Psi_i(x,y)\,dy\,dx, \tag{18}$$

where $\Psi_i(x,y)$ is a solution of Eq. (1) with boundary conditions given by Eq. (3). Differentiation of Eq. (1) with respect to E yields

$$[-m^{-1}\partial^2/\partial x^2 - \partial^2/\partial y^2 + y^2 + V(x-y) - E]\partial\Psi_i(x,y)/\partial E = \Psi_i(x,y). \tag{19}$$

Substitution of this into Eq. (18) gives

$$I = -m^{-1}\int_{-\infty}^{r}\int_{-\infty}^{\infty}\Psi_i^*(x,y)(\partial^2/\partial x^2)[\partial\Psi_i(x,y)/\partial E]\,dy\,dx - \int_{-\infty}^{r}\int_{-\infty}^{\infty}\Psi_i^*(x,y)(\partial^2/\partial y^2)[\partial\Psi_i(x,y)/\partial E]\,dy\,dx + \int_{-\infty}^{r}\int_{-\infty}^{\infty}\Psi_i^*(x,y)[y^2+V(x-y)-E] \times[\partial\Psi_i(x,y)/\partial E]\,dy\,dx. \tag{20}$$

The first integral in Eq. (20) may be integrated by parts twice with the result,

$$\int_{-\infty}^{\infty}\left(\int_{-\infty}^{r}\Psi_i^*(x,y)\frac{\partial^2}{\partial x^2}\frac{\partial\Psi_i(x,y)}{\partial E}\,dx\right)dy = \int_{-\infty}^{\infty}\Psi_i^*(r,y)\frac{\partial}{\partial r}\frac{\partial\Psi_i(r,y)}{\partial E} - \frac{\partial\Psi_i^*(r,y)}{\partial r}\frac{\partial\Psi_i(r,y)}{\partial E}\,dy + \int_{-\infty}^{r}\int_{-\infty}^{\infty}\frac{\partial^2\Psi_i^*(x,y)}{\partial x^2}\frac{\partial\Psi_i(x,y)}{\partial E}\,dy\,dx\ , \tag{21}$$

since it is assumed that $\Psi_i(x,y)$ and its derivative with respect to x vanish at $x=-\infty$. In a similar manner the second integral in Eq. (20) becomes

$$\int_{-\infty}^{r}\left(\int_{-\infty}^{\infty}\Psi_i^*(x,y)\frac{\partial^2}{\partial y^2}\frac{\partial\Psi_i(x,y)}{\partial E}\,dy\right)dx = \int_{-\infty}^{r}\int_{-\infty}^{\infty}\frac{\partial^2\Psi_i^*(x,y)}{\partial y^2}\frac{\partial\Psi_i(x,y)}{\partial E}\,dy\,dx\ . \tag{22}$$

Substituting Eqs. (21) and (22) into Eq. (20) and making use of Eq. (1) yields

$$I = -\frac{1}{m}\int_{-\infty}^{\infty}\Psi_i^*(r,y)\frac{\partial^2\Psi_i(r,y)}{\partial r\partial E} - \frac{\partial\Psi_i^*(r,y)}{\partial r}\frac{\partial\Psi_i(r,y)}{\partial E}\,dy. \tag{23}$$

Since r is assumed large enough that the interaction potential is negligible, the asymptotic form (3) may be used for $\Psi_i(r,y)$ in Eq. (23). This allows the derivatives of $\Psi_i(r,y)$ with respect to r and E to be evaluated explicitly. After much tedious manipulation and use of Eq. (6), the orthonormality of the $\phi_n(y)$, and the conservation of probability,[17]

$$\sum_n P_{ni} = 1\ , \tag{24}$$

one obtains

$$I = r\left(1+\sum_n k_i P_{ni}/k_n\right) + \sqrt{P_{ii}}/k_i\sin(2k_i r+\eta_{ii}) + (2k_i/m)\sum_n P_{ni}(d\eta_{ni}/dE) - (ik_i/m)\sum_n (dP_{ni}/dE)\ . \tag{25}$$

Differentiating Eq. (24) with respect to E yields the identity

$$\sum_n dP_{ni}/dE = 0, \tag{26}$$

which when substituted into Eq. (25) yields the desired result, Eq. (7).

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