Dimensional scaling for quasistationary states

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Complex energy eigenvalues which specify the location and width of quasibound or resonant states are computed to good approximation by a simple dimensional scaling method. As applied to bound states, the method involves minimizing an effective potential function in appropriately scaled coordinates to obtain exact energies in the \( D \to \infty \) limit, then computing approximate results for \( D=3 \) by a perturbation expansion in \( 1/D \) about this limit. For resonant states, the same procedure is used, with the radial coordinate now allowed to be complex. Five examples are treated: the repulsive exponential potential \( (e^{-r}) \); a squelched harmonic oscillator \( (Pe^{-r}) \); the inverted Kratzer potential \( (r^{-1} \text{ repulsion plus } r^{-2} \text{ attraction}) \); the Lennard-Jones potential \( (r^{-12} \text{ repulsion, } r^{-6} \text{ attraction}) \); and quasibound states for the rotational spectrum of the hydrogen molecule \( (X^1\Sigma_g^+, v=0, J=0 \text{ to } 50) \). Comparisons with numerical integrations and other methods show that the much simpler dimensional scaling method, carried to second-order (terms in \( 1/D^2 \)), yields good results over an extremely wide range of the ratio of level widths to spacings. Other methods have not yet evaluated the very broad \( \text{H}_2 \) rotational resonances reported here \( (J>39) \), which lie far above the centrifugal barrier.

I. INTRODUCTION

Systems which can dissociate have a continuous energy spectrum. However, if the dissociation probability is small, the system will have quasistationary states of appreciable lifetime.\(^1\) The energy spectrum then becomes quasidiscrete, consisting of broadened levels with widths inversely proportional to the lifetimes of the transient states. For such quasibound or resonant states, solutions of the Schrödinger equation yield complex eigenvalues; the real and imaginary parts specify, respectively, the position and width of the resonances.

Quasistationary states of atomic and molecular systems have a prominent role in many collisional and spectroscopic processes. Prototype examples include resonances in elastic and inelastic scattering,\(^2\) broadening induced by external fields\(^3\)\(^-\)\(^4\) or inhibited by centrifugal barriers,\(^5\) particularly in rotational predissociation of diatomic molecules.\(^6\) Theoretical methods used to treat resonances likewise exhibit much variety. Aside from direct numerical integration, perhaps the most widely applicable approach is the complex scaling method, also known as the complex coordinate or dilatation transformation method.\(^7\) Other methods or variants include evaluation of poles of the scattering matrix in the complex energy plane,\(^8\) analysis of phase shifts and the collisional time delay,\(^9\) transformations exploiting Lie algebra,\(^10\) and semiclassical techniques.\(^11\)\(^-\)\(^12\)

This paper examines a dimensional scaling treatment which is simple to implement and yields surprisingly accurate results for the positions and widths of resonant states. As with bound states, the method typically involves four steps: (1) generalizing to a space with \( D \) Cartesian dimensions; (2) introducing appropriate \( D \)-scaled coordinates; (3) evaluating exact energies in the \( D \to \infty \) limit, by minimizing an effective potential function; (4) computing approximate results for \( D=3 \) by a perturbation expansion in \( 1/D \) about this limit. For quasibound states, the only special feature is that in steps (3) and (4) the radial coordinate is allowed to be complex. Although dimensional scaling has been chiefly applied to bound states,\(^13\)\(^-\)\(^14\) Popov and co-workers suggested the extension to quasistationary states and obtained good agreement with numerical calculations for short-range power-law, funnel, and Yukawa potentials.\(^15\)\(^-\)\(^16\) They also computed shifts and widths for a hydrogen atom in a strong electric field and in crossed electric and magnetic fields.\(^4\)\(^-\)\(^16\) Here we use an equivalent approach, more directly linked to the complex scaling method,\(^7\) and treat five potentials that offer prototypes for molecular resonances which range from extremely narrow to very broad.

In Sec. II, we formulate the complex dimensional scaling procedure, applicable whether a level is bound or quasibound, or whether located above or below a potential or centrifugal barrier. In Sec. III, we treat the inverted Kratzer potential, which can be solved analytically for both bound and quasibound states, and show that our procedure gives a \( 1/D \) expansion in exact agreement with the analytic solution. In Sec. IV we treat broad resonances in the continuum for three potentials: exponential repulsion, a squelched harmonic oscillator, and Lennard-Jones (12,6). The widths and lifetimes obtained compare well with numerical solutions and with semiclassical quantization. In Sec. V we consider narrow shape resonances for metastable levels of the squelched oscillator well below the barrier top. In Sec. VI we determine the bound and quasibound rotational states of the hydrogen molecule (ground electronic and vibrational state, \( X^1\Sigma_g^+ \) \( v=0 \)) for a wide range of rotational levels \( (J=0 \text{ to } 50) \). Broad resonances not yet evaluated by other methods are included; these resonances \( (J>39, \text{ for } v=0) \) extend far above the centrifugal barrier.
ugal barrier. In Sec. VII prospects for treating many-particle systems are discussed.

II. COMPLEX DIMENSIONAL SCALING

We wish to evaluate complex eigenenergies for a two-body spherically symmetric potential. The radial Schrödinger equation in D dimensions is

$$\frac{1}{2} \frac{d^2}{dr^2} \left( \Lambda(A+1) - 2 \right) + V(r) \right) \Phi(r) = E \Phi(r), \quad (1)$$

where $\Phi(r)$ is the amplitude of the radial probability distribution, with $\int |\Phi|^2 dr = 1$, and units are chosen such that Planck's constant $\hbar$ and the reduced mass are unity. The dimension dependence enters via $\Lambda=I+\frac{1}{2}(D-3)$ and thus simply augments $I$, the orbital angular momentum. The potential $V(r)$ retains the same form as for $D=3$. For a quasibound state the boundary conditions are

$$\Phi(0) = 0, \quad \Phi(r \rightarrow \infty) \sim e^{ikr}, \quad (2)$$

where $k$ is the asymptotic wave number. The corresponding complex eigenenergy,

$$E=E_r - \frac{i}{2} \Gamma \quad (3)$$

specifies the position $E_r$ of the resonance and its width $\Gamma$, inversely proportional to the lifetime of the state.

If the Hamiltonian $H$ for the system is Hermitian, all the eigenenergies are real. However, a non-Hermitian Hamiltonian $H(\theta)$ with complex eigenvalues can be produced by a rotation,

$$H(\theta) = U(\theta) H U^{-1}(\theta), \quad (4)$$

where

$$U(\theta) \Phi(r) = \Phi(re^{i\theta}). \quad (5)$$

The bound states are unaffected by this rotation. The condition that the probability amplitude be square integrable ensures that the resonance positions $E_r$ and widths $\Gamma$ are independent of $\theta$. The resonances appear as poles located below the real energy axis, and from each pole a cut extends downward, subtending an angle of $2\theta$ with respect to the positive axis.

In combination with dimensional scaling, this complex rotation method may be applied either to $D$ or to $r$; we employ the latter option here. For central force problems dimension and angular momentum are isomorphous, as seen in Eq. (1). The appropriate scaling parameter is $\kappa=p+i+\frac{1}{2}(D-1)$, where $p$ is the number of radial nodes. When scaled quantities are ultimately evaluated for $D=3$, this parameter becomes $\kappa=n \equiv p + \frac{1}{2}(D-1)$, the principal quantum number. Accordingly, for central force problems dimensional perturbation expansions in terms of $1/\kappa$ become equivalent to the $1/n$ expansions employed by Popov and co-workers. In this paper, we limit attention to evaluating eigenenergies to second order in a $1/\kappa$ expansion and treat only $p=0$ states. However, other quantities can be computed as well and the perturbation expansions extended to high order, as amply demonstrated for bound state systems.

The basic procedure simply scales distance units by $\kappa^2$ and energy units by $\kappa^{-2}$. Then in the $D \rightarrow \infty$ limit, the radial derivative in Eq. (1) is quenched and the stationary point of the Hamiltonian, at $r=r_0$, is found by minimizing an effective potential $W(r)$, the sum of the scaled centrifugal and potential terms. The eigenenergies can be evaluated by a perturbation expansion about the stationary point,

$$E=E_0 + E_1 \kappa^{-1} + E_2 \kappa^{-2} + \ldots, \quad (6)$$

The leading term $E_0=W(r_0)$, the first-order coefficient $E_1$ is determined by the curvature at $r_0$, and the second-order $E_2$ coefficient by the cubic and quartic derivatives. Explicit expressions are given in the Appendix. For bound states, $r_0$ and the $E_2$ are real; for resonance states complex.

III. AN ANALYTICAL MODEL: KRATZER POTENTIAL

To illustrate the method for a case solvable in closed form, we treat the inverted Kratzer potential. This has been used as a simple model for scattering of electrons from negative atomic ions. The potential, shown in Fig. 1(a), consists of a repulsive Coulomb term and an attractive $r^{-2}$ term,

$$V(r) = \frac{\lambda}{2r^2}$$

where the parameter $\lambda > 0$. At large $r$, the repulsive term is dominant, but at $r=\lambda$ the potential crests at its maximum, $V(\lambda) = 1/(2\lambda)$, and then rapidly plunges to form an attractive well.

When the complex scaling $r \rightarrow re^{i\theta}$ is applied, Eq. (1) becomes

$$\left( \frac{d^2}{dr^2} + \frac{c}{r} + \frac{a}{r^2} \right) \Phi(r) = 0, \quad (8)$$

where

$$a = 2 \kappa^2 e^{i\theta}, \quad b = -2 \kappa e^{i\theta}, \quad c = \lambda - \kappa (\Lambda + 1).$$

The condition that the solution be square integrable requires

$$m^2 - \frac{1}{2} - \frac{b}{2 \sqrt{-a} + 1} = \frac{1}{2} \sqrt{1 - 4e} = 0, \quad (9)$$

where $m=0,1,2,...$. On inserting the values of $a$, $b$, and $c$ we obtain $\theta$-independent complex energy of the form of Eq. (3) with

$$E_r = \frac{\lambda - (m + \frac{1}{2})^2 - (\Lambda + \frac{1}{2})^2}{2[\lambda + (m + \frac{1}{2})^2 - (\Lambda + \frac{1}{2})^2]^2} \quad (10)$$

and

$$\Gamma = \frac{(2m+1)\sqrt{\lambda - (\Lambda + \frac{1}{2})^2}}{[\lambda + (m + \frac{1}{2})^2 - (\Lambda + \frac{1}{2})^2]^2} \quad (11)$$

S. Kais and D. R. Herschbach: Dimensional scaling 3991
To apply the dimensional scaling method to Eq. (1) with the potential of Eq. (7), we introduce scaled units by \( r \rightarrow \kappa^2 r, \lambda \rightarrow \kappa^2 \lambda, E \rightarrow \kappa^2 E \), and obtain

\[
\Phi(r) = E \Phi(r),
\]

with \( \kappa = l + \frac{1}{2}(D-1) \). In the limit \( D \to \infty \), the effective potential becomes

\[
W(r) = \frac{1}{r} + \frac{1-\lambda}{2r^2}.
\]

This has a maximum at \( r_0 = \lambda - 1 \), where \( W(r_0) = \frac{1}{2}(\lambda - 1)^{-1} \). The zeroth-order term in the dimensional perturbation expansion of Eq. (6) is given by \( E_0 = W(r_0) \), as usual. To evaluate higher-order terms, we introduce a complex rotation by \( r \rightarrow \rho = r_0 e^{i\theta}(1 + \kappa^{-1/2} x) \) and expand all quantities in powers of \( \kappa^{-1/2} \). The stationary point of the effective potential with respect to the complex variable \( \rho \) is now at \( \rho_0 = (\alpha - 1)e^{i\theta} \). However, the energy expansion of Eq. (6) depends on the combination \( \rho_0 e^{i\theta} \) and hence is \( \theta \)-independent. For the \( m = 0 \) case, the formulas given in the Appendix yield for the first-order coefficient

\[
E_1 = -\frac{1}{2(\lambda - 1)^2} - i \frac{1}{2(\lambda - 1)^{3/2}}
\]

and for the second-order coefficient

\[
E_2 = \frac{3 - \lambda}{4(\lambda - 1)^3} + \frac{3}{4(\lambda - 1)^{5/2}}.
\]

These expansion coefficients are identical to those obtained by expanding the exact Eqs. (10) and (11) directly in powers of \( \kappa^{-1} \), after introducing the dimension-scaled units, \( \lambda \rightarrow \kappa^2 \lambda \) and \( E \rightarrow \kappa^{-2} E \). This confirms the formal consistency of a dimensional perturbation expansion. Of more practical interest is the accuracy obtained at \( D = 3 \) with just the low-order terms. As illustrated in Fig. 1(b), the accuracy is quite good for both \( E \) and \( \Gamma \), as long as \( \lambda \) is fairly large. This is an intrinsic constraint, since the denominators in the exact expressions require that an expansion in inverse powers of \( \kappa \) also involves inverse powers of \( (\lambda - 1) \). Physically, the constraint arises because as \( \lambda \to 1 \), the stationary point of the effective potential retreats into the origin, \( r_0 \to 0 \).

Although useful for testing formal consistency, the inverted Kratzer potential is extremely atypical because of peculiarities associated with its \( r^{-1} \) and \( r^{-2} \) terms. In contrast to the behavior seen in Fig. 1, usually the width \( \Gamma \) is plotted in Fig. 1(b) for \( m = 0 \) and \( \Lambda = 0 \); merely shifting the abscissa scale to \( M \) gives the results for arbitrary \( \Lambda \neq 0 \). If \( \Delta \lambda \gg (m + \frac{1}{2})^2 \), then \( \Gamma/E \) falls off as \( (\Delta \lambda)^{-1/2} \), whereas in the opposite regime \( \Gamma/E \) grows as \( (m + \frac{1}{2})^2 \).
very broad for resonances above or not far below the barrier top but \( \Gamma \) narrows exponentially as resonances sink below the barrier top.

**IV. BROAD RESONANCES IN THE CONTINUUM**

The complex dimensional scaling method as described above is well suited to evaluating broad resonances, typically with \( \Gamma \) comparable to \( E_r \) for both regular and singular potentials. We simply introduce distance units scaled by \( \kappa^2 \) and energy units scaled by \( \kappa^{-2} \) into Eq. (1), find the corresponding \( k_0 \) for the \( D \to \infty \) effective potential, and evaluate the dimensional expansion coefficients \( E_0, E_1, \) and \( E_2 \). Here we treat three examples in order to compare with results obtained from various other methods.

*A. Exponential repulsive potential*

For this regular and monotonic potential, \( V(r) = Ae^{-r/a} \), no resonances of the usual kind are expected; there are no qualitative features that inhibit separation of collision partners. However, there exist solutions of the radial Schrödinger equation that obey the boundary conditions of Eq. (2) appropriate for quasibound states. \(^{12} \) These have been examined in an S-matrix treatment, \(^{21} \) by semiclassical phase-integral techniques, \(^{22} \) and by numerical integration employing complex rotation of the radial coordinate. \(^{22} \) Table I gives the expansion coefficients we obtained from dimensional scaling. These pertain to the lowest S-wave resonance \( (p=0, l=0) \). For \( D=3 \) (where \( \kappa=1 \)) we compare \( E_T = E_0 + E_1 \) with the accurate numerical results \(^{22} \) given for \( \alpha = 1 \), \( l/2 = 2.4, 2.6, 2.8, \) and 3. The agreement is quite good, within three or four figures for both the resonance positions and widths.

It is noteworthy that, for this case, even the zeroth-order term \( E_0 = W(r_0) \) is complex. This occurs because in the \( D \to \infty \) limit the effective potential has no extremum on the real axis but does have a stationary point in the complex \( r \) plane. Although \( E_0 \), the \( D \to \infty \) energy, gives only a small portion of the real part of the \( D=3 \) energy, it gives the major portion of the resonance width, particularly as the parameter \( A \) increases.

**B. Squelched harmonic oscillator**

This potential is a regular but nonmonotonous function, \( V(r) = V_0(\alpha^2 r^2) e^{-\alpha r} \). It is everywhere non-negative, harmonic for \( r < \alpha \) but exponentially decaying for \( r \geq \alpha \), with a unimodal barrier at \( r = 2\alpha \) of height \( V(2\alpha) = 4V_0\alpha^2 \). An extensive study of this potential has been carried out by Conner and Smith, using numerical integration with complex rotation and comparing results with a uniform semiclassical technique. \(^{17} \) For the lowest resonance \( \Gamma = l=0 \), they give results for \( \alpha = 1 \) and \( V_0 = 1 \) to 20. We consider here the broad resonances with \( V_0 < 4 \) and treat in Sec. V the much narrower resonances found for higher \( V_0 \) values.

Figure 2 plots \( V(r) \) for \( V_0 \) ranging from 0.2 to 20. Also shown are the corresponding effective potentials for the \( D \to \infty \) limit, \( W(r) = 1/r^2 + V(r) \), and the lowest resonances. The broad resonances lie near or above the barrier top, narrow ones well below. We find that simply evaluating the \( D \to \infty \) limit \( E_0 \) and the first-order dimensional perturbation coefficient \( E_1 \) yields good results for the broad resonances. As shown in Table II (for \( V_0 = 1 \)), our results are in agreement with those obtained by Conner and Smith \(^{12} \) from numerical integration, designated \( E_{\text{exact}} \) and is slightly better than that from the uniform semiclassical method, designated \( E_{\text{sc}} \). As with the simple exponential potential, again we find that the \( D \to \infty \) limit yields a complex energy. In this case, however, \( E_0 \) contributes mostly of the real part of the \( D=3 \) energy and little of its width, whereas \( E_1 \) contributes mostly to the width and little to the resonance position.

Figure 3 shows, for \( V_0 \) in the range from 0.7 to 4, how the position \( E_r \) and width \( \Gamma \) of the lowest resonance varies with the barrier height. These curves are again obtained from our first-order \( D \)-scaling approximation, using \( E_T = E_0 + E_1 \). No results are available for comparison in the range \( V_0 < 1 \). In this broad resonance regime, the resonance positions shift steadily upwards with the barrier height, but \( E_r / V_0 \) gradually decreases. The width \( \Gamma \) remains roughly constant as long as the resonance position remains appreciably above the barrier top, but shrinks rapidly when the resonance begins to sink below.

**TABLE I. Expansion coefficients for exponential repulsive potential.**

<table>
<thead>
<tr>
<th>( A )</th>
<th>( E_0 )</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
<th>( E_T )</th>
<th>( E_{\text{exact}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.76</td>
<td>-0.8479 -i5.289</td>
<td>-2.266 +i0.3891</td>
<td>0.0370 +i0.2858</td>
<td>-3.077 -i4.614</td>
<td>-3.064 -i4.615</td>
</tr>
<tr>
<td>6.76</td>
<td>-0.4907 -i6.057</td>
<td>-2.475 +i0.3905</td>
<td>0.0347 +i0.3005</td>
<td>-2.931 -i5.466</td>
<td>-2.917 -i5.466</td>
</tr>
<tr>
<td>7.84</td>
<td>0.0647 -i6.854</td>
<td>-2.668 +i0.1828</td>
<td>0.0324 +i0.3151</td>
<td>-2.719 -i6.3356</td>
<td>-2.703 -i6.355</td>
</tr>
<tr>
<td>9</td>
<td>0.4302 -i7.678</td>
<td>-2.899 +i0.0665</td>
<td>0.0303 +i0.3298</td>
<td>-2.438 -i7.282</td>
<td>-2.421 -i7.280</td>
</tr>
</tbody>
</table>

*From accurate numerical solution (Ref. 20).*

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**TABLE II. Broad resonances for squelched oscillator.**

<table>
<thead>
<tr>
<th>Approx.</th>
<th>( E_r )</th>
<th>( \Gamma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_0 )</td>
<td>0.711 207</td>
<td>0.080 44</td>
</tr>
<tr>
<td>( E_1 )</td>
<td>0.023 16</td>
<td>0.385 54</td>
</tr>
<tr>
<td>( E_T )</td>
<td>0.689 91</td>
<td>0.465 98</td>
</tr>
<tr>
<td>( E_{\text{exact}} )</td>
<td>0.689 4</td>
<td>0.478 6</td>
</tr>
<tr>
<td>( \theta )</td>
<td>0.72 / 4</td>
<td>0.486 0</td>
</tr>
</tbody>
</table>

*For \( \alpha = V_0 = 1 \) and \( n = l = 0 \). Notation specified in text, Sec. IV B.

*From Table II of Ref. 12.*
C. Lennard-Jones potential

As an example of a singular, nonmonotonic potential, we consider the familiar (12,6) potential,

$$V(r) = \epsilon \left[ (\frac{r_m}{r})^{12} - 2 (\frac{r_m}{r})^{6} \right],$$

(19)

where $\epsilon$ denotes the well depth and $r_m$ the radius at the minimum. For the broad resonance regime, accurate results from numerical integration are not available because the outward integration is unstable. However, Conner and Smith have carried out painstaking semiclassical calculations using the two- and three-turning point formulas. Again, we find that the extremely simple first-order dimensional scaling treatment gives results in very good agreement with the much more elaborate semiclassical calculations. Figure 4 compares our resonance positions and
TABLE III. Narrow resonance locations for squelched oscillator.

<table>
<thead>
<tr>
<th>( V_0 )</th>
<th>( E_0 )</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
<th>( E_T )</th>
<th>( E_{\text{exact}}^a )</th>
<th>( E_{\text{approx}}^b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1.9269</td>
<td>0.39587</td>
<td>-0.17529</td>
<td>2.1475</td>
<td>2.1411</td>
<td>2.198</td>
</tr>
<tr>
<td>5</td>
<td>2.2166</td>
<td>0.41839</td>
<td>-0.16656</td>
<td>2.5684</td>
<td>2.5403</td>
<td>2.601</td>
</tr>
<tr>
<td>6</td>
<td>2.4787</td>
<td>0.62849</td>
<td>-0.16392</td>
<td>2.9433</td>
<td>2.9127</td>
<td>2.977</td>
</tr>
<tr>
<td>7</td>
<td>2.7221</td>
<td>0.73066</td>
<td>-0.16362</td>
<td>3.2891</td>
<td>3.2611</td>
<td>3.329</td>
</tr>
<tr>
<td>8</td>
<td>2.9482</td>
<td>0.82377</td>
<td>-0.16439</td>
<td>3.6096</td>
<td>3.5877</td>
<td>3.639</td>
</tr>
<tr>
<td>9</td>
<td>3.1631</td>
<td>0.91645</td>
<td>-0.16570</td>
<td>3.9139</td>
<td>3.8949</td>
<td>3.970</td>
</tr>
<tr>
<td>10</td>
<td>3.3645</td>
<td>1.00168</td>
<td>-0.16729</td>
<td>4.1989</td>
<td>4.1851</td>
<td>4.264</td>
</tr>
<tr>
<td>15</td>
<td>4.2593</td>
<td>1.38353</td>
<td>-0.17631</td>
<td>5.4665</td>
<td>5.4622</td>
<td>5.552</td>
</tr>
<tr>
<td>20</td>
<td>5.0229</td>
<td>1.71335</td>
<td>-0.18497</td>
<td>6.5315</td>
<td>6.5473</td>
<td>6.646</td>
</tr>
</tbody>
</table>

\(^a\)From accurate numerical solution (Ref. 12).
\(^b\)From semiclassical approximation (Ref. 12).

FIG. 3. Position and width of lowest resonance for squelched oscillator potential as functions of parameter \( V_0 \) in the broad resonance regime (cf. Fig. 2). Solid curves obtained from first-order dimensional perturbation treatment; points for \( V_0=1 \) from numerical integrations (Ref. 12). Dashed curve is the locus of the barrier maximum, \( 4V_0/e^2 \).

widths for the \( n=0, l=7, 8, 9, 10 \) states with those of Conner and Smith. Since here \( l=0 \), the first-order energy for \( D=3 \) corresponds to \( E_T = E_0 + E_1 (l+1)^{-1} \). In this case, the \( D-\infty \) limit yields a complex energy which gives comparable contributions to the \( D=3 \) resonance positions and widths.

V. NARROW SHAPE OR TUNNELING RESONANCES

Quasibound states that represent a system temporarily confined by a potential or centrifugal barrier are called shape resonances. Since these states decay by tunneling through the barrier, the widths are often very narrow and depend drastically on the barrier height and breath. In this regime, our dimensional perturbation expansion still provides a simple means to determine the resonance position, \( E_r \). However, other methods are required to obtain the width \( \Gamma \), since the barrier transmission amplitude vanishes more rapidly than any power of \( 1/D \) and hence does not appear in any order of perturbation theory. We return to the squelched oscillator example of Fig. 2, now considering the narrow resonance domain with \( V_0=4 \).

A. Resonance positions

Table III gives the dimensional expansion coefficients for the lowest resonance and the corresponding approximation for the \( D=3 \) energy, \( E_T = E_0 + E_1 + E_2 \), for \( V_0 \) ranging from 4 to 20. Again the agreement with values obtained by direct numerical integration\(^12\) is good; the relative error decreases from 0.3% at \( V_0=4 \) to 0.06% at \( V_0=20 \). This accuracy is appreciably better than found for the semiclassical results derived from the Bohr–Sommerfeld quantization formula.\(^12\) Figure 5 compares the
TABLE IV. Narrow resonance widths for squelched oscillator.

<table>
<thead>
<tr>
<th>$V_0$</th>
<th>$T$</th>
<th>$G$</th>
<th>$\Gamma^a$</th>
<th>$\Gamma_{\text{exact}}^b$</th>
<th>$\Gamma_{\text{sc}}^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>4.6091</td>
<td>0.1516</td>
<td>1.601(-1)</td>
<td>1.760(-1)</td>
<td>1.848(-1)</td>
</tr>
<tr>
<td>5</td>
<td>3.2914</td>
<td>0.4682</td>
<td>1.191(-1)</td>
<td>1.094(-1)</td>
<td>1.161(-1)</td>
</tr>
<tr>
<td>6</td>
<td>2.6337</td>
<td>0.8528</td>
<td>6.897(-2)</td>
<td>6.388(-2)</td>
<td>6.856(-2)</td>
</tr>
<tr>
<td>7</td>
<td>2.2337</td>
<td>1.2582</td>
<td>3.614(-2)</td>
<td>3.514(-2)</td>
<td>3.812(-2)</td>
</tr>
<tr>
<td>8</td>
<td>1.9565</td>
<td>1.6782</td>
<td>8.637(-3)</td>
<td>9.248(-3)</td>
<td>10.22(-3)</td>
</tr>
<tr>
<td>9</td>
<td>1.5950</td>
<td>2.1576</td>
<td>3.196(-6)</td>
<td>3.312(-6)</td>
<td>3.826(-6)</td>
</tr>
<tr>
<td>10</td>
<td>1.1446</td>
<td>4.5447</td>
<td>9.858(-5)</td>
<td>11.63(-5)</td>
<td>13.20(-5)</td>
</tr>
<tr>
<td>15</td>
<td>0.8077</td>
<td>6.4335</td>
<td>3.196(-6)</td>
<td>3.312(-6)</td>
<td>3.826(-6)</td>
</tr>
</tbody>
</table>

$^a$From Eq. (20); number in parentheses is the power of ten by which the entry must be multiplied.

$^b$From accurate numerical solution (Ref. 12).

$^c$From semiclassical approximation (Ref. 12).

TABLE V. Resonances in the ground state of H$_2$ (cm$^{-1}$).

<table>
<thead>
<tr>
<th>$J$</th>
<th>$E_r$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>9 314</td>
<td>752</td>
<td>46</td>
<td>14 559</td>
</tr>
<tr>
<td>41</td>
<td>10 212</td>
<td>1313</td>
<td>47</td>
<td>12 419</td>
</tr>
<tr>
<td>42</td>
<td>11 093</td>
<td>1985</td>
<td>48</td>
<td>16 277</td>
</tr>
<tr>
<td>43</td>
<td>11 966</td>
<td>2751</td>
<td>49</td>
<td>17 134</td>
</tr>
<tr>
<td>44</td>
<td>12 833</td>
<td>3604</td>
<td>50</td>
<td>17 991</td>
</tr>
<tr>
<td>45</td>
<td>13 697</td>
<td>4536</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FIG. 6. Bound ($E_r<0$) and quasibound ($E_r>0$) rotational energy levels (in $10^5$ cm$^{-1}$) for ground state of H$_2$ ($X^1\Sigma_g^+$, $v=0$); curve from first-order dimensional perturbation calculation, points from numerical integration (Ref. 25).

where the $C_n$ coefficients are given by Chan and Dalgarno. Using the composite potential of Eq. (21), Waech and Bernstein computed the complete spectrum of bound and quasibound states, which for $v=0$ extends up to $J=39$, by direct numerical integration of the radial Schrödinger equation.

As shown in Fig. 6, we find that the first order dimensional perturbation calculation (with $\kappa=J+1$) gives good agreement with the numerical results. The mean error is only $\sim0.2\%$ for the bound states and $\sim0.9\%$ for the quasibound or resonance states, with the exception of the levels very near the dissociation asymptote ($J=30$--32). As expected, for those levels the error is larger, from $2\%$--$6\%$. Furthermore, with the dimensional scaling procedure we were able to readily evaluate the positions and widths for the resonances in the continuum above the centrifugal barrier. Table V and Fig. 7 give these results for $v=0$ and $J=40$--50. These resonances, which become very broad as $J$ increases, have not yet been computed by any other method.

VII. DISCUSSION

The complex dimensional scaling procedure offers a remarkably simple means to obtain approximate energy levels. The same procedure is applicable for bound and resonant states. To first order, it requires merely finding the stationary point of an effective potential function and

resonance positions with the maximum in the $D \to \infty$ effective potential.

**B. Resonance widths**

To evaluate $\Gamma$ for these narrow resonances, for simplicity we use the Gamow formula,

$$\Gamma = T^{-1} \exp(-2G),$$

(20)

where $T$ is the period of oscillation within the inner well and $G$ the transmission integral for the barrier,

$$G = \int_{r_1}^{r_2} |k(r)| dr,$n

and $k(r) = \sqrt{2(E-V(r)-(1/8)r^{-2})}$, with $r_0 < r_1 < r_2$ the classical turning points. Table IV compares the $\Gamma$ values thus obtained with those from numerical integration and from the semiclassical (three-point turning point formula) method.12 As $\Gamma$ decreases, the accuracy of the simple Gamow formula improves steadily, and becomes appreciably better than that of the semiclassical method (SC). The Gamow width is too low but its relative error decreases from 10% at $V_0=4$ to 3.7% at $V_0=20$. The SC width is too high and its error increases from 5% to 16% over this range. Figure 5 shows how $\Gamma$ and $\log \Gamma$ vary with the barrier height.

VI. QUASIBOND STATES FOR THE H$_2$ MOLECULE

The very accurate ground state energies for H$_2$ computed by Kolos and Wolniewicz24 have been fitted pointwise by Waech and Bernstein25 to a 33 term polynomial,

$$V(R) = \sum_{n=0}^{32} A_n (R-R_e)^n,$$

(21a)

where $R_e=1.401$ 066 bohr is the equilibrium internuclear distance, $A_0=R_e=38.792$ cm$^{-1}$ the dissociation energy; the higher $A_n$ coefficients are tabulated in Ref. 25. This potential function is accurate to $\pm 1$ cm$^{-1}$ for $R$ up to 4 bohr. There it joins smoothly with a function appropriate for larger $R$, the multipole expansion

$$V(R) = \frac{C_6}{R^6} - \frac{C_8}{R^8} + \frac{C_{10}}{R^{10}}$$

(21b)
a global minimum corresponding to a stable bound state may not exist at \( D \to \infty \) or occur for a markedly nonsymmetrical configuration of the particles. This situation precludes or much complicates the usual approach. Rost shows that complex \( D \) scaling allows the \( 1/D \) perturbation expansion to be developed about the saddle point. In effect, localization there represents a resonance at \( D=\infty \) that correlates with the \( D=3 \) ground state. In this way, Kost obtains for three-body Coulomb systems an analytic first-order result that yields good estimates for the binding energies.

ACKNOWLEDGMENTS

We thank Alex Dalgarno, John Morgan III, and Jan Rost for useful discussions and the Office of Naval Research for support.

APPENDIX: EXPANSION COEFFICIENTS

Here we specify the three-step procedure used to evaluate the expansion coefficients \( E_k \) of Eq. (6), employing notation nearly identical to that of Popov and co-workers.\(^{15,16}\)

1. The classical stationary point, \( r=r_0 \), is determined from the condition

\[
\frac{\nu}{r^\kappa} + \frac{dV}{dr} = 0
\]

as a function of \( \nu \), a scaling parameter; we used \( \nu=\kappa^2 \) with \( \kappa=\nu^{1/2}(D-1) \).

2. The quantities involved in expanding the potential \( V(r) \) about the stationary point are

\[
\begin{align*}
\phi &= \left( \frac{\nu}{r^\kappa} + \frac{dV}{dr} \right)_{r=r_0} \\
\sigma &= 4(1-v_3) \quad \text{and} \quad \tau = \frac{1}{2}(v_4 + \frac{1}{2}).
\end{align*}
\]

Here \( \omega \) represents the harmonic vibrational frequency, \( \sigma \) the cubic, and \( \tau \) the quartic anharmonic constants; these quantities depend on the scaling parameter \( \nu \) by way of \( r_0 \).

3. In the perturbation expansion for the energy,

\[
F = E_0 + E_1 \kappa^{-1} + E_2 \kappa^{-2} + \cdots
\]

the coefficients have the form

\[
E_k = \frac{2\pi \sigma^2}{r_0^4} e_k
\]

where

\[
\begin{align*}
e_0 &= 1 + v_0, \\
e_1 &= (\omega - 1)(2p + 1), \\
e_2 &= \left[ -\frac{3}{4} \omega^{-1} + \frac{1}{4}(\tau + 1) \omega^{-2} + \frac{3}{8} \sigma \omega^{-3} - \frac{11}{6} \omega^{-4} \right] + p(p+1) [1 - 6 \omega^{-1} + (\tau - 1) \omega^{-2} + 6 \sigma \omega^{-3} - \frac{15}{8} \sigma^2 \omega^{-4}] \\
&= \text{etc.}
\end{align*}
\]
Here $p=0,1,2,...$ is the number of radial nodes. Only terms up to $v_k$ in the expansion of the potential contribute to the $E_k$ coefficient.

In their formulation, Popov et al. use $v=n^2/g$, where $g$ is a dimensionless scale factor in the potential. However, in the final expressions for the perturbation coefficients $E_k$, only the combination $g v$ enters; hence Eq. (A4) still holds with $k$ replaced by $n$. Special considerations are required when an energy level is close to zero (i.e., about to become bound or unbound in an attractive potential) or when the harmonic frequency $\omega$ is close to zero (which makes $E_k$ and higher coefficients become singular). Other equivalent formulations have been given by Imbo, Pagnamenta, and Sukhatme and by Mlodinow and Shatz.

The usual $D$-scaling procedure proceeds by introducing $r=k^2\rho$ into Eq. (1) of the text, giving

$$\left[ -\frac{1}{2k^2} \frac{d^2}{dr^2} + \frac{\Lambda(\Lambda+1)}{2k^2r^2} + \kappa^2 V(k^2\rho) \right] \Phi = \kappa^2 E \Phi.$$  \hspace{1cm} (A6)

This makes evident that the appropriate scaling for the energy is $E=\kappa^2\epsilon$. Likewise, for the potential we require $V(k^2\rho)=\kappa^{-2}V(\rho)$, a condition satisfied by simply scaling all dimension parameters by $\kappa$ and all energy parameters by $\kappa^{-2}$. Then, for $\kappa \to \infty$, the scaled radial equation reduces to $\epsilon=\frac{1}{2}\rho^{-2} + V(\rho)$; the condition for a stationary point then yields Eq. (A1) with $v=\kappa^2$, on reverting to the unscaled $r$ coordinate.

Both the $1/n$ expansion of Popov et al. and the $1/k$ expansion used here are semiclassical in character, but differ from the conventional WKB method. In the latter, the classical limit which provides the origin for the perturbation expansion is obtained by $\hbar\to 0$ with the radial quantum number $p\to \infty$ such that $\hbar p=\text{constant}$. With dimensional scaling, $\hbar$ is replaced by $1/D\to 0$, but $p=\text{constant}$, so in effect $\hbar p\to 0$. The origin for the perturbation expansion thus differs from that for the WKB method and therefore the expansion coefficients differ. Usually the WKB method is better for states with large $p$, whereas dimensional scaling is better for low-lying states since in the limit the particle is localized at the minimum of the effective potential. Even for spherically symmetric potential problems, the results may differ substantially, as illustrated in Tables II–IV. For such problems the perturbation expansions reflect differences in the centrifugal terms. The WKB method with the Langer correction has $I(I+1)\to (I+\frac{1}{2})^2$, so the centrifugal term in the effective potential for $I=0$ states is $\frac{1}{2}p^{-2}$, whereas it is $\frac{1}{2}p^{-2}$ for the $D\to \infty$ limit.