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Resonance calculations for arbitrary potentials

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On the basis of model calculations, we argue heuristically that the dilatation-transformation method is applicable to all potentials, even those that are not dilatation analytic. In particular, we show that resonances are converted into bound (localized) states on the nonphysical sheet of the complex energy plane under the action of a dilatation transformation.

I. INTRODUCTION

Resonant scattering is characterized by the energy of the resonance E and the width of the resonance Γ. Taken together, these quantities constitute a complex energy

$$\epsilon = E + \tfrac{1}{2} i \Gamma . \tag{1}$$

Given the Hamiltonian H, the resolvent operator is defined as $(\epsilon - H)^{-1}$. To understand resonant scattering it is necessary to understand the analytic structure of the resolvent operator. The resolvent has poles at real energies corresponding to bound-state eigenvalues of the Hermitian Hamiltonian and cuts along the real axis corresponding to the continuum. Resonances appear as poles of this operator in the complex ϵ plane on the nonphysical energy sheets. That is, the analytic continuation of the resolvent operator through the cuts into the lower half of the complex ϵ plane exhibits poles. The real and imaginary parts of the positions of these poles are interpreted as in (1).

Scattering theory provides a number of ways to find resonance poles. However, in the past several years, a new method[1,2] called the method of *dilatation transformation* (also called the method of complex-coordinate rotations) has been developed which reduces the problem to solving a non-Hermitian eigenvalue problem. This method has been used recently to calculate the resonances[3-9] in electron-atom scattering. We shall see that this new method has many practical advantages over the older scattering methods.

A detailed mathematical justification of the dilatation-transformation method has been given[1,2] for the limited class of so-called dilatation-analytic potentials which includes the many-body Coulomb and Yukawa potentials. However, Reinhardt[10-12] has computed the Stark shift and lifetime of the hydrogen atom using this method and obtained good results even though the potential for the Stark effect is not dilatation analytic (it does not go to zero at infinity). This result suggests that the method is applicable to a wider range of Hamiltonians than one would have previously believed.

The purpose of this paper is to support our belief that the dilatation-transformation method works for all potentials. This includes non-dilatation-analytic local potentials as well as nonlocal potentials such as Hartree-Fock and optical potentials. We do not have a mathematical proof that this method works for such potentials. However, we have successfully applied it to two model problems involving single-particle non-dilatation-analytic potentials, and we have developed a heuristic understanding of how and why it works. We have examined the eigenfunctions corresponding to the resonance eigenvalues of the non-Hermitian eigenvalue problem. We show that this wave function can be interpreted as bound becuase it is localized in character. There are two indications that this interpretation is justified. First, the resonance eigenvalues are isolated; second, they satisfy a complex virial theorem.[13,14] Since bound states satisfy the ordinary virial theorem while continuum (nonlocalized) states do not, this indicates that the resonance wave functions are bound on the nonphysical sheet. In the models we have studied, we find that when this bound eigenfunction is analytically continued back to the physical sheet, it recovers the oscillatory asymptotic behavior expected for a resonance state. Although our model calculations provide the only direct evidence that this is true, we believe that this will be a characteristic result for any potential even if it is not dilatation analytic.

In Sec. II, we briefly dicuss the dilatation-transformation method. In Secs. III and IV, we analyze the cubic anharmonic oscillator and a simple exactly solvable separable nonlocal potential. In Sec. V, we discuss our results and point out some of their implications.

II: DESCRIPTION OF THE DILATATION-TRANSFORMATION METHOD

In 1971, Balslev and Combes[1] showed that a convenient way to perform the analytic continuation to nonphysical sheets in the complex ϵ plane is to use a dilatation transformation

$$\vec{r} \to \vec{r}\, e^{i\theta}, \tag{2}$$

where θ may be real or complex. Transforming the Coulomb Hamiltonian gives, for example,

$$H \to H(\theta) = T(\theta) + V(\theta) = Te^{-2i\theta} + Ve^{-i\theta}, \tag{3}$$

where T and V are the kinetic energy operator and many-body Coulomb potential energy operator. If one solves for the eigenvalue spectrum of a dilatationally transformed Hamiltonian, one finds that[1,2]:

(i) The bound-state eigenvalues remain fixed at their original values along the real axis.

(ii) The continuum eigenvalues are rotated through an angle of -2θ into the lower half of the complex ϵ plane (see Fig. 1). (For simplicity, we consider θ to be a positive real number. For complex θ the angle is $-2\,\mathrm{Re}\,\theta$.)

(iii) When θ becomes large enough, one of the rotated branches passes the position of a resonance pole, and a new eigenvalue of $H(\theta)$ appears at the position (complex energy) of the resonance pole.

(iv) This resonance eigenvalue, once uncovered, remains fixed in the complex ϵ plane and is independent of further increases in θ until θ becomes large enough for another branch to pass through it. At this value of θ, it disappears. In effect, the dilatation transformation fans out the Riemann surface into strips: this allows the resonance poles to appear as complex eigenvalues on the various nonphysical Riemann sheets.

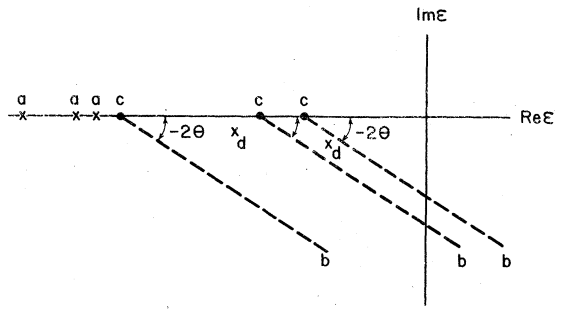

FIG. 1. A schematic view of the eigenvalue spectrum of the dilatationally transformed Hamiltonian $H(\theta)$, showing (a) the bound states, (b) the branch cuts (which extend off to infinity), (c) the continuum thresholds, and (d) the resonance state eigenvalues.

As a practical means of calculating resonances, we expand the transformed Hamiltonian $H(\theta)$ in an appropriately chosen basis set. Then we approximate the exact eigenvalue problem by truncating this basis set. This gives a finite-dimensional-vector-space eigenvalue equation

$$[\underline{H}(\theta) - \epsilon_n(\theta)\underline{I}]\varphi_n(\theta) = 0, \tag{4}$$

which is solved by diagonalizing the non-Hermitian matrix

$$\underline{H}(\theta) = \underline{T}e^{-2i\theta} + \underline{V}e^{-i\theta} \tag{5}$$

(for a Coulomb Hamiltonian). Here, $\underline{T}$ and $\underline{V}$ are the kinetic and potential energy matrices which can be set up using standard bound-state techniques. Note that if the basis is chosen to be independent of θ then these matrices need only be set up once. The resulting finite eigenvalue spectrum of $\underline{H}(\theta)$ is similar to the exact one except that (a) the branch lines appear as a finite set of eigenvalues which rotate by -2θ as a unit (with some scatter due to the finite-basis-set approximation); (b) when one of the branch lines passes through a resonance, one of the eigenvalues detaches itself from the line and remains roughly fixed until it is passed by another branch line, to which it then becomes attached.

Because we have made a finite-basis-set approximation, the position of a resonance eigenvalue is not completely independent of θ. Therefore, we repeat the diagonalization for different values of θ to find that value of θ for which $\epsilon_r(\theta)$ is most nearly stable.[4] This procedure of picking out the most stable value of $\epsilon_r(\theta)$ is usually done graphically. A precise condition for dilatational stability can be obtained[15] by recognizing that the dilatation transformations form a continuous group. The infinitesimal generator of this group is[2,16]

$$A = \vec{r}\cdot\vec{p} + \vec{p}\cdot\vec{r} \tag{6}$$

per particle.

The condition that an eigenvalue be locally invariant under the action of the dilatation group is that the expectation value (with respect to the corresponding eigenfunction) of the commutator of the generator with the Hamiltonian vanish:

$$\langle [A(\theta), H(\theta)\rangle_r = 0, \tag{7}$$

where

$$\langle F(\theta)\rangle_r \equiv \langle \bar{\varphi}_r(\theta), F(\theta)\varphi_r(\theta)\rangle$$

and $\varphi_r(\theta)$ is the solution to

$$[H(\theta) - \epsilon_r(\theta)]\varphi_r(\theta) = 0,$$

while $\bar{\varphi}_r(\theta)$ is the solution to the adjoint equation

$$[H(\theta)^\dagger - \epsilon_r(\theta)^*]\bar{\varphi}_r(\theta) = 0.$$

Equation (7) gives

$$2\langle T(\theta)\rangle_r = \left\langle \sum_i \vec{r}_i \cdot \vec{\nabla}_i V(\theta) \right\rangle_r \tag{8}$$

as the condition for stability. This is just the complex extension of the virial theorem.

III. CUBIC ANHARMONIC-OSCILLATOR MODEL

We have used the dilatation transformation method to identify resonances in the cubic anharmonic oscillator, whose Hamiltonian is given by

$$H = -\frac{d^2}{dx^2} + \frac{x^2}{4} - \lambda x^3, \quad \lambda > 0. \tag{9}$$

This Hamiltonian represents a physical configuration in which a harmonic oscillator is perturbed by a cubic term.

The eigenvalues of the unperturbed ($\lambda = 0$) oscillator are

$$E_n = n + \tfrac{1}{2}, \tag{10}$$

and the eigenfunctions have the form

$$e^{-x^2/4}\mathcal{H}_n(x),$$

where $\mathcal{H}_n(x)$ is a Hermite polynomial.

When $\lambda > 0$, the potential has a well with a minimum at $x = 0$ and a positive maximum at $x = \frac{1}{6}\lambda$. Beyond this barrier, the potential drops off to $-\infty$. The eigenvalue problem for $\lambda \neq 0$ has never been solved in closed form.

We have examined this problem for values of λ for which the height of the potential at its maximum is 1, 2, and 2.5 so that we have one, two, and three resonance states below the potential barrier, respectively. As in the Stark effect,[10-12] the continuum threshold starts at $E = -\infty$. We therefore expect that any value of θ would uncover the resonance states.

We expanded the Hamiltonian in (9) in a basis of the harmonic-oscillator eigenfunctions and diagonalized it. To be sure of our finite-basis-truncation approximation, we repeated our calculation for different values of θ, used different expansion basis sets by using harmonic-oscillator eigenfunctions of the Hamiltonian

$$-\frac{d^2}{dx^2} + \frac{k^2 x^2}{4}$$

for different values of k, and repeated the calculation for increasing basis-set size. We have also calculated the real and imaginary part of the energy for the lowest-energy resonance states (corresponding to the $n = 0$ state) for each of the potentials using a WKB-like matched asymptotic expansion technique described in the Appendix to demonstrate that our results are in fact correct.

A somewhat surprising result of the calculation is that the eigenvalues which make up the continuum do not all rotate smoothly into the lower half plane by -2θ. In fact, some have positive and some have negative imaginary parts. This phenomenon,[17] though surprising at first, can be fairly easily understood. All dilatation-analytic potentials go to zero as $r \to \infty$. Hence, continuum states, being infinite in extent, are dominated by the behavior of the kinetic energy term of the Hamiltonian. Since this transforms as $Te^{-2i\theta}$, one gets the -2θ complex rotation. However, for the cubic oscillator, the potential does not vanish as $x \to \infty$, but in fact diverges like x^3. Hence, the asymptotic behavior of the continuum functions is not dominated by the kinetic energy term, but is determined by a balance between the kinetic and potential energy contributions which rotate in opposite directions.

Despite this difference between the cubic oscillator's transformed eigenvalues and the expected results of a standard dilatation transformation, we do obtain stable converged complex eigenvalues for the resonance states with the correct negative imaginary parts. We obtain resonance states for which Reϵ lies below the potential maximum and also several resonance states for which Re ϵ lies above the potential maximum.

The results of the matrix calculation of the resonance states as well as those of the WKB calculation are presented in Table I. The agreement of the real parts of the energy between the two calculations are very good. The agreement between the imaginary parts improves with decreasing λ to a very good agreement at $\lambda = 0.03$. Since the WKB method becomes better with decreasing λ (see the Appendix), this convergence between the methods shows that the dilatation-transformation matrix calculation has in fact converged to the correct resonance states.

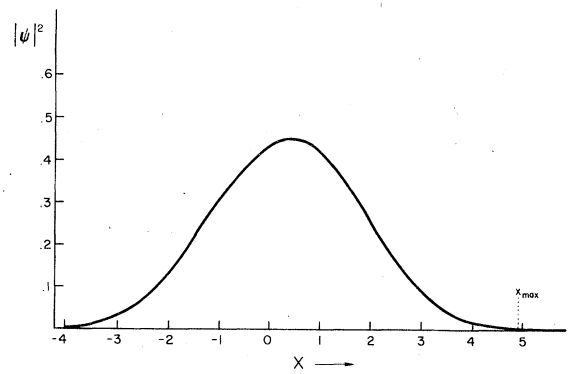

FIG. 2. $|\psi(x)|^2$ for the $n = 0$ state of the anharmonic oscillator with $\lambda = 0.034$ (see Table I). x_{max} is the position of the potential maximum.

TABLE I. Calculated resonance complex eigenvalues for the cubic oscillator.

λ	V_{max}	n [b]	Matrix [a] Reϵ	$-$Imϵ	WKB Reϵ [c]	$-$Imϵ [c]	% discrepancy Re	Im
0.0481 [d]	1.0005	0	0.465 9(9)	2.280(2) $\times 10^{-3}$	0.4746	3.085×10^{-3}	1.86	35.3
		1	1.250(9)	0.112(2)	...	...	...	...
0.034 [e]	2.0002	0	0.485 693 7(1)	2.875(5) $\times 10^{-6}$	0.4873	3.214×10^{-6}	0.33	11.8
		1	1.391 574 8(3)	1.341 7(7) $\times 10^{-2}$	...	...	...	...
		2	2.818(1)	0.363 9(1)	...	...	...	...
		3	3.59(1)	0.77(2)	...	...	...	...
0.03 [e]	2.572	0	0.491 947 1(1)	5.93(12) $\times 10^{-8}$	0.4901	6.03×10^{-8}	0.38	1.69
		1	1.422 922 6(1)	4.092(1) $\times 10^{-5}$	...	...	...	...
		2	2.225 019 5(5)	7.408(3) $\times 10^{-3}$	...	...	...	...
		3	2.923 4(1)	0.139 10(6)	...	...	...	...
		4	3.618 2(7)	0.468(3)	...	...	...	...

[a] The matrix results are the average of all of the runs at the largest size matrix diagonalized. The error is the average deviation from the average.

[b] The corresponding harmonic-oscillator quantum number.

[c] Calculated from Eq. (A5).

[d] Calculated using three 20×20 runs in single precision: $k = 0.5$, $\theta = 0.2$ rad; $k = 0.5$, $\theta = 0.5$ rad; $k = 1.0$, $\theta = 0.2$ rad.

[e] Calculated using four 40×40 runs in double precision: $k = 0.4$, $\theta = 0.1$ rad; $k = 0.4$, $\theta = 0.2$ rad; $k = 0.7$, $\theta = 0.1$ rad; $k = 0.7$, $\theta = 0.2$ rad.

To investigate the boundedness properties of the resonance wave functions on the nonphysical sheet, we have looked at $|\psi_r(x)|^2$. These are plotted in Figs. 2–4 for the $n = 0, 1, 2$ states of the $\lambda = 0.034$ potential. The plots definitely shows that the functions are localized. The exponential falloff of the wave functions, which continues smoothly far beyond the region depicted in the graphs, is not caused by the exponential decay in the basis set. This is checked by examining the continuum functions to see when the exponential falloff sets in. The $n = 0$ resonance wave function looks very much like a harmonic-oscillator wave function, slightly shifted towards positive x and slightly distorted by compressing the function at negative x and expanding it towards positive x. The full width at half maximum corresponds to an $n = 0$ harmonic-oscillator function with a k of about 0.8. One calculation was done in a $k = 0.7$ basis set. (The projection of this wave function on the $n = 0$, $k = 0.7$ harmonic-oscillator wave function is 0.957.) The $n = 1$ resonance wave function again resembles the $n = 1$ harmonic-oscillator wave function, but, as one would expect from a state higher up in the potential well, it is more compressed at negative x and more elongated at positive x. It is composed mostly of the $n = 1$ harmonic-oscillator wave function ($|c_1|^2 = 0.813$) with

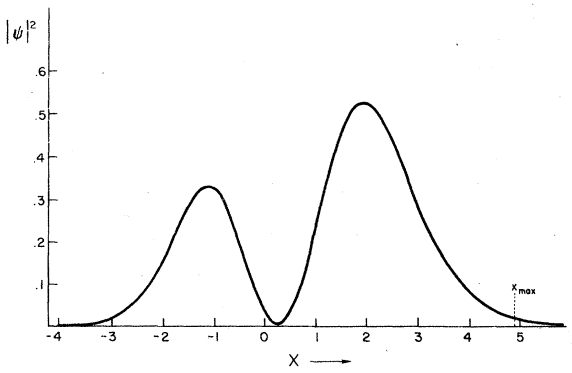

FIG. 3. $|\psi(x)|^2$ for the $n = 1$ state of the anharmonic oscillator with $\lambda = 0.034$ (see Table I). x_{max} is the position of the potential maximum.

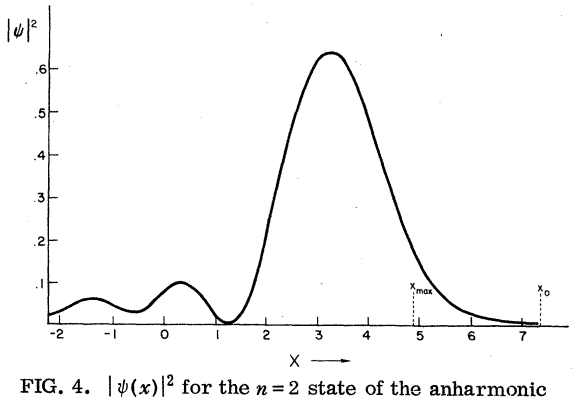

FIG. 4. $|\psi(x)|^2$ for the $n = 2$ state of the anharmonic oscillator with $\lambda = 0.034$ (see Table I). x_{max} and x_0 are the positions of the potential maximum and the zero in the potential, respectively.

some $n=2$ ($|c_2|^2=0.127$) mixed in. The $n=2$ resonance state lies above the potential maximum and it is even more distorted towards positive values of x.

IV. SEPARABLE-POTENTIAL MODEL (REF. 18)

The eigenvalue problem

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{\mathbf{r}})+\int d\vec{\mathbf{r}}'V(\vec{\mathbf{r}},\vec{\mathbf{r}}')\psi(\vec{\mathbf{r}}')=E\psi(\vec{\mathbf{r}}) \quad (11)$$

corresponds to a particle of mass m moving in a *nonlocal* potential. The usual *local* eigenvalue problem is recovered when the nonlocal potential has the form

$$V(\vec{\mathbf{r}},\vec{\mathbf{r}}')=V(\vec{\mathbf{r}})\delta(\vec{\mathbf{r}}-\vec{\mathbf{r}}'). \quad (12)$$

The change in the kinetic energy operator under the dilatation transformation has been discussed above. It will be assumed that the transformation of the nonlocal potential carries Eq. (12) into

$$-(\hbar^2/2m)e^{-2i\theta}\nabla^2\psi(\vec{\mathbf{r}})+e^{3i\theta}\int d\vec{\mathbf{r}}'\,V(\vec{\mathbf{r}}e^{i\theta},\vec{\mathbf{r}}'e^{i\theta})\psi(\vec{\mathbf{r}}')=E\psi(\vec{\mathbf{r}}). \quad (13)$$

Here, all the position variables have been transformed by $\vec{\mathbf{r}}\to\vec{\mathbf{r}}e^{i\theta}$, including those associated with integration over $\vec{\mathbf{r}}'$. When $V(\vec{\mathbf{r}},\vec{\mathbf{r}}')$ is actually local [of the form of Eq. (12)], we recover (4).

When the potential $V(\vec{\mathbf{r}},\vec{\mathbf{r}}')$ is separable,

$$V(\vec{\mathbf{r}},\vec{\mathbf{r}}')=\lambda U(|\vec{\mathbf{r}}|)U(|\vec{\mathbf{r}}'|) \quad (14)$$

closed-form solutions are easily obtained. For this special case, Eq. (13) becomes

$$-(\hbar^2/2m)e^{-2i\theta}\nabla^2\psi(\vec{\mathbf{r}})+C(\theta)U(re^{i\theta})=E\psi(\vec{\mathbf{r}}), \quad (15)$$

where

$$C(\theta)=e^{3i\theta}\lambda\int d\vec{\mathbf{r}}'\,U(r'e^{i\theta})\psi(\vec{\mathbf{r}}'). \quad (16)$$

Because of the spherical symmetry of Eq. (15), the energy eigenfunctions $\psi(\vec{\mathbf{r}})$ can also be chosen to be angular momentum eigenfunctions. For all $l>0$ states, (16) yields $C(\theta)=0$, so the solutions are just free-particle states. Only the $l=0$ states (s waves) are not free. When $l=0$, $\psi(\vec{\mathbf{r}})$ may be written

$$\psi(\vec{\mathbf{r}})=f(r)/r, \quad (17)$$

where $f(r)$ is determined by the one-dimensional problem

$$\left(E+\frac{\hbar^2}{2m}e^{-2i\theta}\frac{d^2}{dr^2}\right)f(r)=C(\theta)rU(re^{i\theta}), \quad (18)$$

$$C(\theta)=4\pi\lambda e^{3i\theta}\int_0^\infty dr\,rU(re^{i\theta})f(r). \quad (19)$$

The general solution to the inhomogeneous problem (18) is

$$f(r)=Ae^{ikr}+Be^{-ikr}+\frac{2me^{2i\theta}C(\theta)}{k\hbar^2}\int_0^r dx\,xU(xe^{i\theta})\sin k(r-x) \quad (20)$$

with $k^2=2mEe^{2i\theta}/\hbar^2$. We choose k so that Im $k<0$. If $U(r)$ has a finite range, then

$$f(r)\underset{r\to\infty}{\sim}\left(A+\frac{me^{2i\theta}C(\theta)}{i\hbar^2k}\int_0^\infty dx\,xU(xe^{i\theta})e^{-ikx}\right)e^{ikr}+\left(B-\frac{me^{2i\theta}C(\theta)}{i\hbar^2k}\int_0^\infty dx\,xU(xe^{i\theta})e^{ikx}\right)e^{-ikr}. \quad (21)$$

The condition that the state be bound is equivalent to the condition that the coefficient of e^{ikr} in (21) be zero. This determines the constant of integration A. We also impose a second boundary condition $f(0)=0$ so that $\psi(r)$ will not be too singular at the origin. The solution satisfying these conditions is

$$f(r)=-\frac{2me^{2i\theta}C(\theta)}{\hbar^2k}\times\left(e^{-ikr}\int_0^r dx\,xU(xe^{i\theta})\sin kx+\sin kr\times\int_r^\infty dx\,xU(xe^{i\theta})e^{-ikx}\right). \quad (22)$$

Equation (22) represents a bound-state solution to (18). The consistency relation (19) remains to be imposed. With (22), this is equivalent to the relation

$$1=-\frac{8\pi m\lambda e^{5i\theta}}{\hbar^2k}\int_0^\infty dr\,rU(re^{i\theta})\times\left(e^{-ikr}\int_0^r dx\,xU(xe^{i\theta})\sin kx+\sin kr\int_r^\infty dx\,xU(xe^{i\theta})e^{-ikx}\right). \quad (23)$$

In general this is a transcendental equation in k. Those solutions with Im $k<0$ correspond to bound states.

If $U(r)=e^{-br}/r$, the integration in (23) is readily performed and the result is quite simple:

$$1=-\frac{4\pi m\lambda}{b\hbar^2(b+ike^{-i\theta})^2}, \quad (24)$$

with $\cos\theta>0$ necessary for the convergence of the integrals. This is just a quadratic relation in k. If $\lambda>0$, the two solutions are

$$k=[ib\pm(1/\hbar)(4\pi m\lambda/b)^{1/2}]e^{i\theta}. \quad (25)$$

The corresponding complex energy

$$E = 2\pi\lambda/b - \hbar^2 b^2/2m \pm 2i\hbar(\pi b\lambda/m)^{1/2} \quad (26)$$

is independent of θ, as expected from the virial-theorem argument.[13,14]

A solution with both Im $E < 0$ and Im $k < 0$ occurs only if

$$\theta > \tan^{-1}[\hbar b^{3/2}/(4\pi m\lambda)^{1/2}]. \quad (27)$$

Thus, a finite rotation is required to produce a bound-state solution.

With (27) satisfied, (22) gives an analytical representation to the eigenfunction. This function is readily analytically continued to $\theta = 0$. At $\theta = 0$ the asymptotic r dependence is

$$f(r) \sim e^{-ikr}; \quad -ik = b + (i/\hbar)(4\pi m\lambda/b)^{1/2}. \quad (28)$$

As θ decreases below the critical value in (27), the bound, exponentially decaying state $f(r)$ analytically continues into an exponentially growing state. This is the behavior of a true resonance state, so this transition conforms to the general expectation: the analytic continuation of the bound state, determined with (27) satisfied, represents a true resonance state and the eigenvalue represents the actual resonance energy.

For $\lambda < 0$, Eq. (24) gives

$$k = i[b \pm (1/\hbar)(4\pi m\,|\lambda|/b)^{1/2}]e^{i\theta} \quad (29)$$

and an Im $k < 0$ solution

$$k = i[b - (1/\hbar)(4\pi m|\lambda|/b)^{1/2}]e^{i\theta} \quad (30)$$

occurs when

$$-\lambda > b^3\hbar^2/(4\pi m). \quad (31)$$

This represents a bound state with real energy

$$E = -\frac{\hbar^2 b^2}{2m}\left[1 - \frac{1}{b\hbar}\left(\frac{4\pi m|\lambda|}{b}\right)^{1/2}\right]^2, \quad (32)$$

which is again independent of θ. This state is present for all θ when Eq. (31) is satisfied and no resonance state is present. In the intermediate case, $\lambda < 0$ but (31) not satisfied, there is neither a bound state nor a resonance.

The transformations $r \to re^{-i\theta}$, $x \to xe^{-i\theta}$ in the general relation (23) which fixes k show that it is actually an equation for $ke^{-i\theta}$. It is thus generally true that the eigenvalues E do not vary with θ. The k values do vary with θ because the solutions of (23) are of the form $ke^{-i\theta} = \text{const}$. Thus, the solutions of (23) may be pictured as rotations by an angle $-\theta$ of complex numbers k with Im $k < 0$. When rotated back to $\theta = 0$, the resulting analytically continued eigenfunction will behave for large r like e^{ikr} and therefore resemble a resonance state. For the separable model (14), then, bound states of the rotated-eigenfunction problem are equivalent to resonance states of the original problem.

V. DISCUSSION

The results of these model calculations plus those of Reinhardt[10-12] strongly suggest that the dilatation-transformation method is applicable to any resonance-scattering problem, both for local and nonlocal potentials. While these examples do not constitute a mathematical proof, it is our feeling that enough examples have been done to assure us that the method has a large (and probably universal) domain of applicability and that it ought to be applied to real physical problems of current interest.

Our results lead to a description of a resonance as a localized eigenfunction on a nonphysical sheet of the complex energy plane. These results, and our previous demonstration that the complex virial theorem is the necessary and sufficient condition for dilatational stability, lead to the following picture of the dilatation transformation and resonances: At $\theta = 0$, the bound states satisfy the virial theorem and hence do not move under the action of the transformation. The continuum states do not satisfy the virial theorem and, thus, rotate by -2θ and fan out on the Riemann surface. When a branch passes through a resonance, a new localized state appears on a nonphysical sheet with a complex energy corresponding to the resonance. Since it satisfies the virial theorem, it is effectively a bound state and it remains stable until is is covered up.

There is a particular problem which can occur in one dimension (but can be avoided in higher-dimensional problems) when the potential does not become strongly positive for negative (or positive) x, such as in the quartic oscillator $V(x) = x^2 - \lambda x^4$. While we expect that the resonance wave function should become bound on the nonphysical sheets, this clearly will not happen if we use the transformation $x \to xe^{i\theta}$. This is true because if we find a θ such that $\psi_r(x, \theta)$ is exponentially decreasing for positive x it will be exponentially increasing for negative x. Hence, to obtain localized resonance states on the nonphysical sheet, one should replace the transformation with something like

$$x \to x e^{i\theta \operatorname{sgn} x}.$$

For one-sided potentials such as the cubic oscillator, this is unnecessary because the repulsive nature of the potential for negative x will insure exponentially decreasing wave functions as $x \to -\infty$ independent of the dilatation transformation. This problem is avoided in more than one dimension by using spherical coordinates where the potential is

always one-sided (r ranges from 0 to ∞).

Strictly speaking, the dilatation transformation in N dimensions applied to the vector $\vec{\mathbf{r}}=(r, \varphi_1, \varphi_2, \cdots, \varphi_{N-1})$ takes the form

$$\vec{\mathbf{r}} \to (re^{i\theta}, \varphi_1, \varphi_2, \cdots \varphi_{N-1}) .$$

Thus, when $N>1$ we can always express $\vec{\mathbf{r}}$ in terms of positive numbers (angles and distances). The problem in one dimension is that x can be either positive or negative.

Knowing that the resonance wave function is bound on the nonphysical sheets suggests different strategies for choosing basis sets in their calculation. That is, we want to find a wave function $\psi_r(\vec{\mathbf{r}}, \theta)$ which is bound for some θ for which the resonance is uncovered. If we know the approximate position of the resonance eigenvalue (as we frequently do from experiment or approximate calculations) and if we know the approximate positions of the relevant continuum branch thresholds (as we frequently do), we can choose a range of θ such that the resonance will be uncovered. Choosing a value of θ somewhere in the center of such a range to perform the calculation, we can tailor the basis set to give us bound-state-like wave functions at the desired θ. Of course, any intuition about the shape of the resonance wave function should be put into this choice of basis. One place this seems especially useful is in the scattering off a system (atom) with inner electronic shells. Since the inner shells are only slightly affected by the scattering process, one expects that the description of the inner shells on the nonphysical sheet should be almost the same as their description on the physical sheet for a free noninteracting system. This expectation can be built into the basis set when one knows the dilatation angle. This is most readily done by recognizing that the wave function on the nonphysical sheet of a "true bound" state is obtained from the wave function on the physical sheet by just making the substitution $\vec{\mathbf{r}}_i \to \vec{\mathbf{r}}_i e^{i\theta}$ in the wave function as has been pointed out by Junker and Huang[8] and Rescigno and coworkers.[9] Hence, following their suggestion, one includes such functions in the basis for the inner-core electrons by obtaining them from a standard (good) atomic calculation. The rest of the basis would then only have to correct the inner-core electronic wave function for the inadequacies of this "frozen core" approximation. This would allow most of the basis set to be used for the evaluation of the outer shells and the scattering-particle part of the resonance wave function rather than having to be used to undo the effect of the dilatation transformation on the inner shells. By such tailoring of the basis set, the convergence properties of the calculation are improved and the necessity of going to very large basis sets is minimized. One can then use the complex virial theorem to monitor the convergence as the basis set is increased while keeping the dilatation angle constant. Of course, such basis-set tailoring will require a considerable amount of calculational experimentation, but the knowledge that the resonance wave function is bound can not fail to be of help in this effort.

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APPENDIX

In this Appendix we show how to calculate the real and the imaginary parts of the eigenvalues of the Schrödinger equation

$$\left(\frac{-d^2}{dx^2}+\frac{x^2}{4}-\lambda x^3-E(\lambda)\right)y(x)=0 . \tag{A1}$$

For small λ we may treat $H_{\text{int}}=-\lambda x^3$ as a perturbation. The eigenvalue $E(\lambda)$ can be represented by

$$E=\mathrm{Re}E+i\,\mathrm{Im}E .$$

The corrections to ReE take the form of a power series in λ:

$$\mathrm{Re}E=n+\tfrac{1}{2}+\sum_{n=1}^{\infty}A_n\lambda^n .$$

The first-order correction to ReE vanishes because H_{int} is an odd function of x:

$$\int_{-\infty}^{\infty}dx\,|y_n|^2H_{\text{int}}=\lambda\sum_{-\infty}^{\infty}dx\,[e^{-x^2/4}\mathcal{H}_n(x)]^2x^3=0 .$$

Thus, the first nonvanishing correction to ReE is of order λ^2. We calculate ReE to second order in λ by expanding both the eigenvalue and the eigenfunction in a power series in λ. We consider just the ground state. First we let

$$E(\lambda)=\tfrac{1}{2}+A\lambda^2 .$$

We know that any corrections from ImE will be *exponentially* small and will not affect this calculation. Next, we let

$$y(x)=W(x)e^{-x^2/4} .$$

The function $W(x)$ represents the anharmonic corrections to the wave function. Differentiating gives

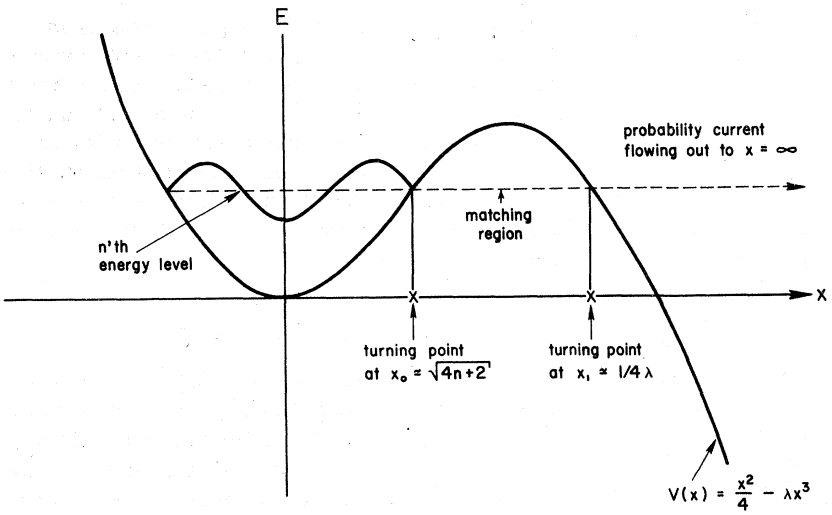

FIG. 5. The anharmonic-oscillator potential.

$$y' = (-\tfrac{1}{2}xW + W')e^{-x^2/4},$$

$$y'' = [(\tfrac{1}{4}x^2 - \tfrac{1}{2})W - xW' + W'']e^{-x^2/4}.$$

Substituting into (A1) gives

$$-W'' + xW' - \lambda x^3 W - A\lambda^2 W = 0.$$

Finally, we represent $W(x)$ as a perturbation series in powers of λ:

$$W = 1 + \lambda(ax + bx^3) + \lambda^2(cx^2 + dx^4 + ex^6) + \cdots.$$

Equating powers of λ gives

$$\lambda': \quad -6bx + ax + bx^3 - x^3 = 0,$$

whence

$$b = \tfrac{1}{3}, \quad a = 2;$$

$$\lambda^2: \quad -2c - 12dx^2 - 30ex^4 + 2cx + 4dx^4 + ex^6 - ax^4 - bx^6 - A = 0,$$

whence

$$e = \tfrac{1}{18},$$

$$c = \tfrac{11}{2},$$

$$d = \tfrac{11}{12},$$

$$A = -11.$$

Hence,

$$\mathrm{Re}E(\lambda) = \tfrac{1}{2} - 11\lambda^2 + O(\lambda^4). \qquad \text{(A2)}$$

It is known that this series, which is the series that one obtains from conventional perturbation theory, is asymptotic to ReE. Note again that the corrections to ImE vanish exponentially as $\lambda \to 0$ and therefore do not appear in this calculation. There may, of course, be exponentially small terms in the expansion of ReE. However, such terms are subdominant and negligible in the present context.

Now, we compute ImE following the procedure described in Ref. 19. We use the fact that ImE is proportional to the flow of probability current J out to infinity as depicted in Fig. 5. To solve the problem we use asymptotic matching. For $0 \leq x \leq \frac{1}{4}\lambda$, we approximate (A1) by

$$\left(\frac{-d^2}{dx^2} + \frac{x^2}{4} - E(\lambda)\right)y = 0,$$

whose solution up to normalization is just the parabolic-cylinder functions

$$y(x) = D_n(x). \qquad \text{(A3)}$$

For $1 \ll x < 1/4\lambda$, we use WKB theory to solve Eq. (A1). Then we match both solutions together to obtain the probability current.

The probability current is

$$J(x) = \frac{1}{2i}\left(-y^*(x)\frac{dy(x)}{dx} + y(x)\frac{dy^*(x)}{dx}\right).$$

It must be normalized by dividing by

$$\int_{-\infty}^{\infty} dx\,|y(x)|^2 \simeq \int_{-\infty}^{\infty} dx\, D_n^2(x) = (2\pi)^{1/2} n!.$$

We therefore have

$$I_m E = J(x)/(2\pi)^{1/2} n!,$$

where the right-hand side is evaluated at any value $x \geq 1/4\lambda$, the right-most turning point of the potential.

The asymptotic matching goes as follows: The WKB approximation is given by

$$y(x)_{\mathrm{WKB}} = C_1(x^2 - 4\lambda x^3 - 4n - 2)^{-1/4} \times \exp\left(-\int_{x_0}^{x} dt\,(\tfrac{1}{4}t^2 - \lambda t^3 - n - \tfrac{1}{2})^{1/2}\right).$$

By matching to $D_n(x)$ we obtain

$$C_1 = \exp\{\tfrac{1}{2}(n+\tfrac{1}{2})[\ln(n+\tfrac{1}{2})-1]\} .$$

We now substitute y_{WKB} into the expression for J and obtain simply

$$\mathrm{Im}E = -\frac{C_1^2 e^{-2I}}{2(2\pi)^{1/2} n!} , \tag{A4}$$

where

$$I = \int_{x_0}^{x_1} dt\,(\tfrac{1}{4}t^2 - \lambda t^3 - n - \tfrac{1}{2})^{1/2} .$$

Here we have chosen to evaluate $J(x)$ precisely at $x = 1/4\lambda$.

It remains only to calculate the integral I and we are done. We evaluate I by considering it in each of two regions:

$$\begin{aligned} I &= \int_{(4n+2)^{1/2}}^{1/4\lambda} dx\,(\tfrac{1}{4}x^2 - \lambda x^3 - n - \tfrac{1}{2})^{1/2} \\ &= \frac{1}{2}\int_{(4n+2)^{1/2}}^{1/4\lambda} dx\,(x^2 - 4\lambda x^3 - 4n - 2)^{1/2} \\ &= \tfrac{1}{2}I_1 + \tfrac{1}{2}I_2 \\ &= \frac{1}{2}\int_{(4n+2)^{1/2}}^{\alpha} dx\,(x^2 - 4\lambda x^3 - 4n - 2)^{1/2} \\ &\quad + \frac{1}{2}\int_{\alpha}^{1/4\lambda} dx (x^2 - 4\lambda x^3 - 4n - 2)^{1/2} , \end{aligned}$$

where α is an arbitrary intermediate point $(4n+2)^{1/2} \ll \alpha \ll 1/4\lambda$. Evaluating the integrals yields

$$I_1 = (n+\tfrac{1}{2})\ln(4n+2) - n - \tfrac{1}{2} - 2(n+1)\ln(2\alpha) + \cdots ,$$

and

$$I_2 = 1/60\lambda^2 + (2n+1)\ln(\lambda\alpha) + \cdots .$$

Combining I_1 and I_2 gives

$$I = \tfrac{1}{2}\{1/60\lambda^2 - n - \tfrac{1}{2} + (n+\tfrac{1}{2})\ln[\lambda^2(n+\tfrac{1}{2})]\} .$$

Observe that α has dropped out, as it should.

Now we substitute into (A4):

$$C_1^2 = \exp\{(n+\tfrac{1}{2})[\ln(n+\tfrac{1}{2}) - 1]\} .$$

Hence, after a little algebra

$$\mathrm{Im}E = -\frac{\exp(-1/60\lambda^2)\lambda^{-2n-1}}{2(2\pi)^{1/2} n!} .$$

Thus, for the lowest level, $n = 0$, we have

$$E = \tfrac{1}{2} - 11\lambda^2 - i\,\frac{\exp(-1/60\lambda^2)}{2(2\pi)^{1/2}\lambda} + \cdots . \tag{A5}$$

Note added in proof. In this note we argue that the positive imaginary eigenvalues of the cubic anharmonic oscillator which make up the continuum as we rotate into the complex plane are actually an artifact of the limited basis which was used for the numerical calculations. Indeed, a reexamination of these states using larger basis sets indicates that the transformed continuum contribution moves *down* in the complex plane as the basis is increased. Similar behavior was found for the dilatationally transformed Stark problem by Reinhardt and co-workers (private communication, Reinhardt). Here is a heuristic argument which shows that under an infinitesimal rotation the continuum eigenvalues move down in the complex ϵ plane to $-i\infty$.

We approximate the exact continuum wave function $\Psi(\epsilon)$ of real energy ϵ by a square integrable function $u(\epsilon)$. Since the behavior of the wave function is dominated by the asymptotic region as $x \to \infty$ the cubic oscillator Hamiltonian (9) can be replaced by

$$T - \lambda x^3 , \quad \lambda > 0$$

without any loss of generality.

The result of an infinitesimal dilatation transformation $x \to xe^{i\delta}$ upon the state approximated by $u(\epsilon)$ is given in first-order perturbation theory as

$$\epsilon(\delta) = -2i\delta\langle u(\epsilon), Tu(\epsilon)\rangle - 3i\delta\lambda\langle u(\epsilon), x^3 u(\epsilon)\rangle .$$

As we let $u(\epsilon)$ become a better approximation to $\Psi(\epsilon)$,

$$-\lambda\langle u(\epsilon), x^3 u(\epsilon)\rangle \to -\infty$$

as $u(\epsilon) \to \Psi(\epsilon)$.

However,

$$\langle u(\epsilon), Tu(\epsilon)\rangle - \lambda\langle u(\epsilon), x^3 u(\epsilon)\rangle = \epsilon_u \to \epsilon ,$$

(a finite number) as $u(\epsilon) \to \Psi(\epsilon)$.

Thus,

$$\langle u(\epsilon), Tu(\epsilon)\rangle \to +\infty$$

as $u(\epsilon) \to \Psi(\epsilon)$.

Hence,

$$\epsilon(\delta) \to -i\infty$$

as $u(\epsilon) \to \Psi(\epsilon)$

independently of δ.

While this demonstration cannot be taken to the limit, it does indicate strongly that the continuum spectrum of the dilatationally transformed cubic oscillator is *empty*. This demonstration is similar to a proof (using a different method) of Reinhardt and co-workers that the continuum spectrum of the dilatationally transformed Stark problem is empty

(private communication, Reinhardt). If the above method is used on the Stark problem it also gives $\epsilon(\delta) \to -i\infty$. However, when it is applied to a dilatation analytic potential where $V(x) \to 0$ as $x \to \infty$ it yields the familiar -2δ rotation of the continuum cut.

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