Intrinsic relationship between dynamical resonance energy and decay rate

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In the framework of dilatation transformation based on complex scaling, we show that the dilated non-Hermitian Hamiltonian may be decoupled into two separated Hermitian operators, namely, the resonance energy operator and the decay rate operator, i.e., the FWHM. We present an intrinsic relationship between these operators. Specifically, we show that the effective potential for resonance decay rate is a virial function of the effective potential for resonance energy. As examples of their application, we invoke the decoupled Hamiltonian operators for resonance states of a single particle in a central force field and to problems in potential scattering to identify the resonance states and determine resonance energy and decay rate.

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I. INTRODUCTION

In contrast to bound states, quasibound states, i.e., dynamical resonances, are characterized by states with a relative stability but a finite lifetime. These states are ubiquitous and clearly some of the most important dynamical processes [1–4], including reaction dynamical resonances such as quantum transition state resonances and reaction thresholds [5–7]. Quantum dynamical resonance states also play a key role in optimal and optical control of molecular dynamics [8].

Among the various approaches to studies of quasibound states, the rigged Hilbert space theory is one of the most successful [9]. Mathematically, it is generated by a dilatation transformation of the basic Hilbert space by extending the reaction coordinates into a complex domain, i.e., $r \to r e^{i\theta}$, such that a dilatation-transformed, diagonalizable, non-Hermitian system Hamiltonian $\hat{H}(r e^{i\theta})$ is obtained.

The development of the theory has been encouraging, and many numerical applications have been successful by invoking the complex virial theorem [9–27], which was first analyzed by Balslev and Combes [9]. These researchers provided a mathematical foundation for the complex virial theorem that can be written in a variational form, i.e., $dE(\theta)/d\theta = 0$. Further discussions on the complex virial theorem of quasistationary molecular systems were given by Tachibana *et al.* and others [28–33]. Throughout the years, the rigged Hilbert space theory has been applied to various quantum dynamical processes, e.g., atomic and molecular physics, chemical reaction dynamics, etc.

In summary of the rigged Hilbert space theory, a complex dilated system Hamiltonian has the following physical features and mathematical advantages:

(i) A quantum reaction dynamical process is generally an unbound scattering process and contains a mixture of bound-unbound states. In such a case, the wave function is generally not square integrable. With the complex dilatation transformation, the rigged Hilbert space wave function becomes square integrable, i.e., an L^2 function. Mathematically, it behaves exactly like that of a bound-state wave function. Because the wave function becomes square integrable, the eigenvalue problem may be performed to obtain energies and eigenfunctions, in exactly the same way as that of a bound state.

(ii) The bound-state eigenvalues are not affected by the complex dilatation transformation. In other words, the bound-state eigenvalues are not changed regardless of the transformation.

(iii) The continuum states in scattering processes are filtered out as background. They do not have any effects on the dynamical process, nor do they have any mathematical implication on numerical calculation.

(iv) Each quasibound state (resonance) embedded in the continuum will distinguish itself in providing a complex eigenvalue for the complex scaled Hamiltonian, $E(\theta) = E_R(\theta) - i\Gamma(\theta)/2$, where $E_R(\theta)$ is the resonance energy and $\Gamma(\theta)$ is the FWHM. For a given scaling parameter θ, the resonance lifetime is related to its FWHM such that $\tau(\theta) = \hbar/\Gamma(\theta)$.

(v) The scaling parameter θ is obtained by the so-called complex virial theorem, $dE(\theta)/d\theta = 0$, to determine the corrected resonance states with corresponding resonance energies and lifetimes.

In this paper, we show that the dilatation-transformed non-Hermitian Hamiltonian operator can be formally decoupled into two interrelated Hermitian operators, namely, the resonance energy operator and resonance width operator [18]. We present a theoretical derivation of an intrinsic relationship between the aforementioned operators, i.e., an intrinsic relationship between resonance energy $E_R(\theta)$ and its FWHM $\Gamma(\theta)$. To illustrate this intrinsic relationship and the practical calculations of quasibound states, we apply the decoupled Hamiltonian operators to problems in potential scattering and resonance states of a single particle in a central force field.

II. RELATIONSHIP BETWEEN RESONANCE ENERGY AND DECAY RATE

For a quantum reactive dynamical process, dilatation transformation of Hilbert space is generated by complex scaling of the reaction coordinate in basic Hilbert space [9], obtained by replacement of the reaction coordinate via the transformation $r \to r e^{i\theta}$. This operation is achieved through a unitary dilatation transformation $\hat{U}(\theta) = e^{i\theta\hat{S}}$, where $\hat{S} = i(r\hat{p} + \hat{p}r)/2\hbar$ is the so-called generating operator. By noting

that momentum $\hat{p} = -i\hbar(d/dr)$, we may write the generating operator in the form of the virial operator,

$$\hat{S} = \frac{1}{2}\left(r\frac{d}{dr} + \frac{d}{dr}r\right). \qquad (1)$$

Application of the dilatation transformation $\hat{U}(\theta)$ to a wave function, $\psi(r,\theta) = \hat{U}(\theta)\psi(r)$, yields

$$\psi(r,\theta) = e^{i\theta/2}\psi(re^{i\theta}). \qquad (2)$$

This rigged Hilbert space wave function now becomes square integrable (L^2 function) and behaves similarly to that of the bound-state wave function.

The dilated Hamiltonian operator is given by

$$\hat{H}(re^{i\theta}) = \hat{U}(\theta)\hat{H}(r)\hat{U}(\theta)^{-1}, \qquad (3)$$

which, sometimes denoted by $\hat{H}(r,\theta) = \hat{H}(re^{i\theta})$, becomes a non-Hermitian operator that can be used to characterize quasibound states with finite lifetimes. Correspondingly, its real part represents the center of a resonance energy and its imaginary part is interpreted as the rate of resonance decay. By solving the eigenvalue equation

$$\hat{H}(r,\theta)\psi(r,\theta) = E(\theta)\psi(r,\theta), \qquad (4)$$

it yields the resonance energy and resonance FWHM, $E(\theta) = E_R(\theta) - i\Gamma(\theta)/2$.

It can be shown that the dilated Hamiltonian operator can be decoupled into a real and an imaginary part [14] as expressed by

$$\hat{H}(r,\theta) = \hat{H}_R(r,\theta) - i\frac{1}{2}\hat{\Gamma}(r,\theta). \qquad (5)$$

For a given system with potential function $V(r)$, by defining $V_0(r) = V(r)$, and

$$V_n(r) = -\frac{1}{2}r\frac{d}{dr}V_{n-1}(r), \quad n = 1,2,\ldots \qquad (6)$$

the operator for resonance energy takes the form

$$\hat{H}_R(r,\theta) = \cos(2\theta)\frac{\hat{p}^2}{2\mu} + \left[V_0(r) - \frac{(2\theta)^2}{2!}V_2(r)\right.$$
$$\left. + \frac{(2\theta)^4}{4!}V_4(r) - \cdots\right]$$
$$= \cos(2\theta)\frac{\hat{p}^2}{2\mu} + \sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k}}{(2k)!}V_{2k}(r), \qquad (7)$$

while the operator for resonance width is given by

$$\frac{1}{2}\hat{\Gamma}(r,\theta) = \sin(2\theta)\frac{\hat{p}^2}{2\mu} + \left[\frac{(2\theta)^1}{1!}V_1(r) - \frac{(2\theta)^3}{3!}V_3(r)\right.$$
$$\left. + \frac{(2\theta)^5}{5!}V_5(r) - \cdots\right]$$
$$= \sin(2\theta)\frac{\hat{p}^2}{2\mu} + \sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k+1}}{(2k+1)!}V_{2k+1}(r). \qquad (8)$$

Now, if we define the effective potential functions $U(r,\theta)$ and $W(r,\theta)$ such that

$$U(r,\theta) = \sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k}}{(2k)!}V_{2k}(r) \qquad (9)$$

and

$$W(r,\theta) = \sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k+1}}{(2k+1)!}V_{2k+1}(r), \qquad (10)$$

we may write the resonance energy operators as

$$\hat{H}_R(r,\theta) = \cos(2\theta)\frac{\hat{p}^2}{2\mu} + U(r,\theta), \qquad (11)$$

$$\frac{1}{2}\hat{\Gamma}(r,\theta) = \sin(2\theta)\frac{\hat{p}^2}{2\mu} + W(r,\theta). \qquad (12)$$

The significance of the pair of operators in Eqs. (11) and (12), each acting as an effective Hamiltonian operator, is that they are Hermitian operators and represent resonance energy and resonance width (i.e., decay rate).

The interrelationship between the operators $\hat{H}_R(r,\theta)$ and $\hat{\Gamma}(r,\theta)$ is of interest to us. In order to obtain a better understanding, we examine $U(r,\theta)$ and $W(r,\theta)$ in greater detail. In the following discussion, we show that the effective potential function $W(r,\theta)$ is a virial function of $U(r,\theta)$. Conversely, $U(r,\theta)$ can also be written as a virial function of $W(r,\theta)$. It is exactly this mutual virial relationship between $U(r,\theta)$ and $W(r,\theta)$ that provides us with an improved understanding of the complex virial theorem.

First, we write $W(r,\theta)$ as a virial of $U(r,\theta)$. By invoking the condition given in Eq. (6), we can write $W(r,\theta)$ such that

$$W(r,\theta) = \sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k+1}}{(2k+1)!}V_{2k+1}(r)$$
$$= -\frac{1}{2}r\frac{d}{dr}\left[\sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k+1}}{(2k+1)!}V_{2k}(r)\right]. \qquad (13)$$

Taking the first derivative of $W(r,\theta)$ in Eq. (13) with respect to θ gives

$$\frac{d}{d\theta}W(r,\theta) = -r\frac{d}{dr}\left[\sum_{k=0}^{\infty}\frac{(-1)^k(2\theta)^{2k}}{(2k)!}V_{2k}(r)\right] \qquad (14)$$

or

$$\frac{d}{d\theta}W(r,\theta) = -r\frac{d}{dr}U(r,\theta). \qquad (15)$$

Thus we may write $W(r,\theta)$ in terms of $U(r,\theta)$ as

$$W(r,\theta) = \int_{\theta}\left[-r\frac{d}{dr}U(r,\eta)\right]d\eta. \qquad (16)$$

Equation (16) shows that the effective potential for resonance width $W(r,\theta)$ is fundamentally the virial function of $U(r,\theta)$ that acts as an effective potential for the energy operator $\hat{H}_R(r,\theta)$. We can then readily rewrite Eq. (12) as

$$\frac{1}{2}\hat{\Gamma}(r,\theta) = \sin(2\theta)\frac{\hat{p}^2}{2\mu} + \int_{\theta}\left[-r\frac{d}{dr}U(r,\eta)\right]d\eta. \qquad (17)$$

Using the trigonometric identity

$$\sin(2\theta) = 2\int_{\theta}\cos(2\eta)d\eta, \qquad (18)$$

we have

$$\hat{\Gamma}(r,\theta) = 4\int_{\theta}\left[\cos(2\eta)\frac{\hat{p}^2}{2\mu} - \frac{1}{2}r\frac{d}{dr}U(r,\eta)\right]d\eta. \qquad (19)$$

Equations (11) and (19) are the central result of this letter. They indicate that the effective potential for resonance decay rate, as given in Eq. (19), is a virial function of the effective potential for resonance energy, shown in Eq. (11). Both operators are Hermitians which, for a given dynamical system, can be used to determine its quasibound states.

III. BOUND STATES

As the first example, let us consider a bound state, a simple one-dimensional harmonic oscillator with potential $V(x) = m\omega^2 x^2/2$ and $\psi(-\infty) = \psi(\infty) = 0$. Even though this is a trivial case, it somewhat illustrates the relationship discussed in Eq. (19). Invoking Eq. (6), we have

$$V_0(x) = V_2(x) = V_4(x) = V_{2j}(x) = \tfrac{1}{2}m\omega^2 x^2, \quad j = 1,2,3,\ldots \tag{20}$$

Then,

$$U(x,\theta) = \sum_{k=0}^{\infty} \frac{(-1)^k (2\theta)^{2k}}{(2k)!} \left(\frac{1}{2}m\omega^2 x^2 \right)$$

$$= \cos(2\theta)\left(\frac{1}{2}m\omega^2 x^2 \right), \tag{21}$$

$$\frac{1}{2}x\frac{d}{dx}U(x,\theta) = \cos(2\theta)\left(\frac{1}{2}m\omega^2 x^2 \right). \tag{22}$$

Applying Eqs. (21) and (22) to Eqs. (10) and (17) yields

$$\hat{H}_R(x,\theta) = \cos(2\theta)\left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right), \tag{23}$$

$$\hat{\Gamma}(x,\theta) = 2\sin(2\theta)\left(\frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2 x^2 \right). \tag{24}$$

The complex virial theorem requires $dE(\theta)/d\theta = 0$, which means

$$\frac{d}{d\theta}\langle \hat{H}(x,\theta)\rangle = \frac{d}{d\theta}\langle \hat{H}_R(x,\theta)\rangle - i\frac{1}{2}\frac{d}{d\theta}\langle \hat{\Gamma}(x,\theta)\rangle = 0. \tag{25}$$

Equivalently, this gives us

$$\frac{d}{d\theta}\langle \hat{H}_R(x,\theta)\rangle = -2\sin(2\theta)\left\langle \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right\rangle$$

$$= 0 \rightarrow \theta = 0, \tag{26}$$

$$\frac{d}{d\theta}\langle \hat{\Gamma}(x,\theta)\rangle = 4\cos(2\theta)\left\langle \frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2 x^2 \right\rangle = 0 \rightarrow \theta = \frac{\pi}{4}. \tag{27}$$

For $\theta = 0$,

$$E_R = \left\langle \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right\rangle = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0,1,2,\ldots, \tag{28}$$

$$\Gamma = 2\sin(2\theta)\left\langle \frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2 x^2 \right\rangle_{\theta=0} = 0. \tag{29}$$

This is exactly the normal result for a harmonic oscillator in quantum mechanics, where ω is the oscillator frequency.

For $\theta = \pi/4$,

$$E_R = \cos(2\theta)\left\langle \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right\rangle_{\theta=\pi/4} = 0, \tag{30}$$

$$\frac{\Gamma}{2} = \sin(2\theta)\left\langle \frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2 x^2 \right\rangle_{\theta=\pi/4}$$

$$= \left\langle \frac{\hat{p}^2}{2m} + \frac{1}{2}m\,(i\omega)^2\,x^2 \right\rangle = \left(n + \frac{1}{2}\right)\hbar\,(i\omega). \tag{31}$$

Thus the total system energy is given as

$$E = E_R - i\frac{1}{2}\Gamma = \left(n + \frac{1}{2}\right)\hbar\omega, \tag{32}$$

and it is clear that the $\theta = \pi/4$ scaling likewise does not change the physical nature of the system. As expected, dilatation transformation with complex scaling does not alter any physical properties of a bound state. In this case, it is a simple harmonic oscillator.

Let us consider a generic bound value problem with the system Hamiltonian $\hat{H}(r) = \hat{p}^2/2\mu + V(r)$, where $V(r)$ is an arbitrary potential well. With a scaling parameter $0 \leqslant \theta < \pi/2$, let us define an effective mass $m(\theta) = \mu/\cos(2\theta)$. The resonance energy and width operators can then be written as

$$\hat{H}_R(r,\theta) = \frac{\hat{p}^2}{2m(\theta)} + U(r,\theta), \tag{33}$$

$$\hat{\Gamma}(r,\theta) = 4\int_{\theta}\left[\frac{\hat{p}^2}{2m(\eta)} - \frac{1}{2}r\frac{d}{dr}U(r,\eta) \right]d\eta. \tag{34}$$

Invoking the complex virial theorem for resonance energy, $d\langle \hat{H}(r,\theta)\rangle/d\theta = 0$, we have for the resonance energy

$$\frac{d}{d\theta}\langle \hat{H}_R(r,\theta)\rangle = \frac{d}{d\theta}\left\langle \frac{\hat{p}^2}{2m(\theta)} + U(r,\theta) \right\rangle = 0. \tag{35}$$

Equation (35) can be solved to provide a critical scaling parameter θ_c, from which we can obtain a resonance energy

$$E_R = \left\langle \frac{\hat{p}^2}{2m(\theta_c)} + U(r,\theta_c) \right\rangle. \tag{36}$$

Application of the complex virial theorem to the decay rate operator yields

$$\frac{d}{d\theta}\langle \hat{\Gamma}(r,\theta)\rangle = 4\left\langle \frac{\hat{p}^2}{2m(\theta)} - \frac{1}{2}r\frac{d}{dr}U(r,\theta) \right\rangle = 0. \tag{37}$$

It is obvious that the scaling parameter θ_c obtained from Eq. (35) is also a solution for Eq. (37), due to the fact that

$$2\left\langle \frac{\hat{p}^2}{2m(\theta_c)} \right\rangle = \left\langle r\frac{d}{dr}U(r,\theta_c) \right\rangle. \tag{38}$$

Therefore, using Eq. (34), $\Gamma = 0$.

It is clear that for a bound state, the real part of the energy is restored to its value before scaling and the decay rate is zero. Thus complex scaling indeed does not alter any system dynamics for bound states.

IV. SCATTERING STATES

To illustrate the case of unbound states, we now discuss the resonances in scattering over a potential barrier. Again, let us first consider a simple parabolic potential barrier $V(x) = -m\omega^2 x^2/2$ for which $\psi(-\infty)$ and $\psi(\infty)$ are free states.

Using Eq. (6) we have

$$V_0(x) = V_2(x) = V_4(x) = V_{2j}(x)$$
$$= -\frac{1}{2}m\omega^2 x^2, \; j = 1,2,3,\ldots \quad (39)$$

Then

$$U(x,\theta) = \sum_{k=0}^{\infty} \frac{(-1)^k (2\theta)^{2k}}{(2k)!} \left(-\frac{1}{2}m\omega^2 x^2\right)$$
$$= -\cos(2\theta)\left(\frac{1}{2}m\omega^2 x^2\right), \quad (40)$$

$$\frac{1}{2}x\frac{d}{dx}U(x,\theta) = -\cos(2\theta)\left(\frac{1}{2}m\omega^2 x^2\right), \quad (41)$$

and

$$\hat{H}_R(x,\theta) = \cos(2\theta)\left(\frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2 x^2\right), \quad (42)$$

$$\hat{\Gamma}(x,\theta) = 2\sin(2\theta)\left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2\right). \quad (43)$$

It should be noted that the complex scaled Hamiltonian $\hat{H}(x,\theta)$ has square-integrable eigenfunctions, which provide Eqs. (42) and (43) with the boundary conditions $\psi(-\infty,\theta) = \psi(\theta,\infty) = 0$.

Using the complex virial theorem for $d\Gamma(\theta)/d\theta = 0$ leads to

$$\frac{d}{d\theta}\langle\hat{\Gamma}(x,\theta)\rangle = 4\cos(2\theta)\left\langle\frac{\hat{p}^2}{2\mu} - \frac{1}{2}m\omega^2 x^2\right\rangle = 0 \rightarrow \theta = \frac{\pi}{4}. \quad (44)$$

Therefore,

$$\frac{1}{2}\Gamma = \sin(2\theta)\left\langle\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2\right\rangle_{\theta=\pi/4} = \left(n + \frac{1}{2}\right)\hbar\omega, \quad (45)$$

$$E_R = \cos(2\theta)\left\langle\frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2 x^2\right\rangle_{\theta=\pi/4} = 0. \quad (46)$$

Equations (45) and (46) represent the well-known resonance state for the parabolic potential barrier with resonance lifetime $\tau = 2\hbar/\Gamma = 2/(2n+1)\omega$ and a maximum resonance lifetime $\tau = 2/\omega$.

For an arbitrary potential barrier $V(r)$, the system Hamiltonian may be written as $\hat{H}(r) = \hat{p}^2/2\mu + V(r)$. The scaled potential barrier is effectively

$$U(r,\theta) = V(r) + \sum_{k=1}^{\infty} \frac{(-1)^k (2\theta)^{2k}}{(2k)!} V_{2k}(r). \quad (47)$$

Because the potential in Eq. (47) has a barrier, its virial function as given below, practically, has a potential well,

$$\frac{d}{d\theta}W(r,\theta) = -r\frac{d}{dr}U(r,\theta). \quad (48)$$

With a scaling parameter, $0 \leqslant \theta < \pi/2$, and an effective mass defined by $m(\theta) = \mu/\cos(2\theta)$, the resonance energy and width operators can be written as

$$\hat{\Gamma}(r,\theta) = 4\int_\theta \left[\frac{\hat{p}^2}{2m(\eta)} - r\frac{d}{dr}U(r,\eta)\right]d\eta, \quad (49)$$

$$\hat{H}_R(r,\theta) = \frac{\hat{p}^2}{2m(\theta)} + U(r,\theta). \quad (50)$$

Application of the complex virial theorem to the decay rate operator yields

$$\frac{d}{d\theta}\langle\hat{\Gamma}(r,\theta)\rangle = 4\left\langle\frac{\hat{p}^2}{2m(\theta)} - \frac{1}{2}r\frac{d}{dr}U(r,\theta)\right\rangle = 0, \quad (51)$$

which determines a critical scaling parameter θ_c and guarantees the regular virial theorem. Solving the eigenvalue problem for the resonance width operator $\hat{\Gamma}(r,\theta_c)$, which has a effective potential well $W(r,\theta)$, yields a proper resonance wave function. The resonance energy is then calculated by

$$E_R = \left\langle\frac{\hat{p}^2}{2m(\theta_c)} + U(r,\theta_c)\right\rangle. \quad (52)$$

Thus potential barrier scattering provides a potential well for the resonance width operator that can be used to determine the corresponding resonance wave function and resonance lifetime.

V. A SINGLE PARTICLE IN A CENTRAL FORCE POTENTIAL FIELD

As a final consideration, we now discuss the case of a single particle in the field of a central force potential $V(r)$. By spherical coordinates, the system Hamiltonian takes the form

$$\hat{H}(\mathbf{r}) = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\mathbf{L}^2}{2mr^2} + V(r), \quad (53)$$

where $\mathbf{L}$ is the angular momentum operator. The eigenfunctions are of the form

$$\Psi(\mathbf{r}) = \frac{1}{r}\psi_\ell(r)Y_{\ell m}(\theta,\phi). \quad (54)$$

Using Eqs. (53) and (54), it yields a one-dimensional Schrödinger equation for the central potential,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + V(r)\right]\psi(r) = \mathrm{E}\psi(r). \quad (55)$$

For a fixed angular moment ℓ, Eq. (55) provides an effective central potential:

$$V_{\mathrm{eff}}(r) = \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + V(r). \quad (56)$$

This effective potential, for a given angular momentum ℓ, is within the group of arbitrary potential barriers that can be dilated to obtain information on resonance states, as

discussed earlier. Theoretically, the discussion above holds for all states with or without angular momentum ℓ, provided that $\lim\limits_{r\to 0} r^2 V(r) = 0$.

Now, let us consider a practical anharmonic central force potential in the special case of $\ell = 0$, namely, an inverted Morse potential barrier [18],

$$V(x) = D_e[2e^{-\alpha x} - e^{-2\alpha x}], \qquad (57)$$

where α is a Morse potential parameter and $x = r - r_e$ is the distance from the barrier height, $r = r_e$, with $D_e > 0$. In this case, the function related to resonance width is practically a potential well given by

$$\begin{aligned} W(x,\theta) &= \sum_{k=0}^{\infty} \frac{(-1)^k (2\theta)^{2k+1}}{(2k+1)!} V_{2k+1}(x) \\ &= D_e \alpha^2 x^2 \sin(2\theta) + \sum_{k=1}^{\infty} \frac{(-1)^k (2\theta)^{2k+1}}{(2k+1)!} \\ &\quad \times (ax^3 + bx^4 + cx^5 + \cdots). \end{aligned} \qquad (58)$$

With the defined problem above, the particle is trapped inside the well and the boundary conditions are given by $\psi(-r_e) = \psi(\infty) = 0$. An eigenvalue problem can be solved for this potential well to obtain the resonance width:

$$\langle \psi_n | \sin(2\theta) \frac{\hat{p}^2}{2\mu} + W(x,\theta) | \psi_n \rangle = \frac{1}{2} \Gamma_n(\theta). \qquad (59)$$

Under harmonic approximation, with standard $\theta = \pi/4$ as for the harmonic oscillator, Eq. (59) leads to

$$\Gamma_n = 2\left(n + \frac{1}{2}\right)\hbar \sqrt{\frac{2D_e\alpha^2}{\mu}}, \quad n = 0,1,2,\ldots. \qquad (60)$$

The resonance energy may then be calculated by

$$\begin{aligned} E_{R,n} &= \langle \psi_n | \cos(2\theta) \frac{\hat{p}^2}{2\mu} + U(x,\theta) | \psi_n \rangle_{\theta=\pi/4} \\ &= D_e - \frac{1}{4D_e}\left(n + \frac{1}{2}\right)^2 \hbar^2 \left(\sqrt{\frac{2D_e\alpha^2}{\mu}}\right)^2, \\ & \qquad n = 0,1,2,\ldots \end{aligned} \qquad (61)$$

Equations (60) and (61) are again the well-known solutions of resonance states for the inverted anharmonic Morse oscillator.

For $\ell \neq 0$, we write the centrifugal barrier term as

$$u(r) = \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2}. \qquad (62)$$

It is easy to verify that

$$-\frac{1}{2} r \frac{d}{dr} u(r) = \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} = u(r), \qquad (63)$$

$$u_0(r) = u_1(r) = \cdots = u_n(r) = \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} = u(r), \\ n = 1,2,3,\ldots. \qquad (64)$$

Then, for the effective potential $V_{\text{eff}}(r)$, as given in Eq. (56), we have

$$\begin{aligned} W(x,\theta) &= \sum_{k=0}^{\infty} \frac{(-1)^k (2\theta)^{2k+1}}{(2k+1)!} (V_{\text{eff}})_{2k+1}(x) \\ &= \sin(2\theta)\left[D_e\alpha^2 x^2 + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{(x+r_0)^2}\right] \\ &\quad + \sum_{k=1}^{\infty} \frac{(-1)^k (2\theta)^{2k+1}}{(2k+1)!}(ax^3 + bx^4 + \cdots). \end{aligned} \qquad (65)$$

Under harmonic approximation, it can be written as

$$\begin{aligned} W(x,\theta) &= \sum_{k=0}^{\infty} \frac{(-1)^k (2\theta)^{2k+1}}{(2k+1)!} (V_{\text{eff}})_{2k+1}(x) \\ &\approx \sin(2\theta)\left[D_e\alpha^2 x^2 + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r_0^2}\right]. \end{aligned} \qquad (66)$$

Equation (66) provides a resonance state with decay rate of

$$\Gamma_n = (2n+1)\hbar \sqrt{\frac{2D_e\alpha^2}{\mu} + \frac{\hbar^2}{m} \frac{\ell(\ell+1)}{r_0^2}}, \quad n = 0,1,2,\ldots. \qquad (67)$$

VI. DISCUSSION

Alternative approaches, both different from and similar to the dilatation transformation based on complex scaling, have also been successful for finding resonances in atomic and molecular dynamics. A stationary principle for quantum resonance states, separate from dilatation transformation by complex scaling, was developed by Truhlar and Mead [5]. In that formalism, a generalized antiunitary operator was proposed for a generalized dilatation transformation (GDT) in terms of time reversal. Truhlar and Mead showed that the time-reversal operator provided a stationary formulism for finding resonances in atomic and molecular systems, and discussed the difference and similarity between the Truhlar-Mead stationary principle and the method of complex dilatation. Actually, for the complex scaled Hamiltonian as discussed in this paper, its eigenvalues can also be obtained by the Truhlar-Mead principle [5] in seeking stationary points of

$$E(\theta) = \frac{\langle \widehat{C}\Psi(r) | \hat{H}(r,\theta) | \Psi(r) \rangle}{\langle \widehat{C}\Psi(r) | \Psi(r) \rangle}. \qquad (68)$$

In Eq. (68), $\widehat{C}$ is an antiunitary operator and $\Psi(r)$ is a trial function for stationary points.

Specifically, in the method of dilatation transformation based on complex scaling, for systems of a single particle in a central force potential field, the resonance-state expectation values are calculated by

$$E(\theta) = \frac{\langle \psi^*(r,\theta) | \hat{H}(r,\theta) | \psi(r,\theta) \rangle}{\langle \psi^*(r,\theta) | \psi(r,\theta) \rangle}, \qquad (69)$$

where $\psi^*(r,\theta)$ is a complex conjugate of $\psi(r,\theta)$. Examining Eqs. (68) and (69), we recognize that

$$\widehat{C}\psi(r,\theta) = \psi^*(r,\theta). \qquad (70)$$

It is worth noting that for the examples discussed in this paper, under harmonic approximation, the eigenfunctions are real, i.e., the eigenfunctions are not complex functions. Therefore we have $\psi^*(r,\theta) = \psi(r,\theta)$, and

$$E(\theta) = \frac{\langle \psi^*(r,\theta)|\hat{H}(r,\theta)|\psi(r,\theta)\rangle}{\langle \psi^*(r,\theta)|\psi(r,\theta)\rangle}$$
$$= \frac{\langle \psi(r,\theta)|\hat{H}(r,\theta)|\psi(r,\theta)\rangle}{\langle \psi(r,\theta)|\psi(r,\theta)\rangle}. \quad (71)$$

In summary, we have presented an intrinsic relationship between resonance energy and resonance width in the framework of dilatation transformation by complex scaling. We show that the dilated non-Hermitian Hamiltonian operator can be formally decoupled into two interrelated Hermitian operators, corresponding to resonance energy and resonance decay rate, and that the decoupled operators can be applied successfully to determine dynamical resonances. Although the applications are limited to the simplest cases in this paper, the theory is generalizable to any dynamical system. We expect that more successful applications of the theory to practical, complex, multidimensional problems will be forthcoming.

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