Weyl's theory and the complex-rotation method applied to phenomena associated with a continuous spectrum

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Weyl's theory for a singular second-order differential equation and the complex scaling method of Balslev and Combes are combined to obtain a stable method for describing the continuous spectrum. The method obtained can be viewed as an extension of the Siegert method. The theory is applied to a model potential earlier used by Moiseyev et al.

The experimental development of laser spectroscopy, electron scattering, and in particular, the high-frequency deflection technique,[1] have lead to a considerable interest in the theory of the spectral continuum and more specifically in quasibound states and resonances in the vibrational continua of molecules. The simultaneous development of complex scaling in terms of the Aguilar-Balslev-Combes (ABC) theory[2-4] for dilatation analytic operators has opened a field of new ideas. Methods of this type are important for the understanding of a complete, nonisolated system.

One of the first applications of the ABC theory in the study of resonances was reported by Bain, Bardsley, Junker, and Sukumar.[5] They used a modified variational principle to obtain the complex eigenvalue of the complex-rotated Hamiltonian. The position of the resonance as a function of the dilatation angle was studied numerically. One of the difficulties of the application of this method is its basis-set dependence. This problem was to some extent solved utilizing the existence of the complex virial theorem.[6]

Weyl's theory for a singular second-order differential equation[7] has earlier proven to be an efficient tool in the analysis of the continuous spectrum.[8] In the numerical applications made so far (see, e.g., Hehenberger et al.[9] and Ref. 8) one makes use of the numerical information of the Green's function or the Weyl-Titchmarsh m function on the real axis. A Siegert state[10] can then only be obtained via analytic continuation based on the previously mentioned numerical data.

In this report we present a synthesis of Weyl's theory and the theory of complex scaling. The step to "go into" the complex plane appears, in fact, quite natural if the details of Weyl's theory are considered. In contrast to previous techniques which one way or another were based on the numerical dependence of the resonance solutions on the dilatation angle $\theta = \arg \eta$, we employ a direct numerical integration of the Siegert[10] solution on the higher-order Riemann sheet. As a consequence, the dependence of the resonances on $\theta = \arg \eta$ is essentially eliminated, in agreement with the Balslev-Combes theorem.[2-4] An additional benefit of this approach, when considering Weyl's theory, is that we avoid the ansatz of the analytic continuation.

Our synthesis can be viewed as an extension of the Siegert method[10] in the sense that, in addition to relating the eigenvalue to the complex boundary condition, we also make the coordinates complex so as to make the wave function square integrable. This is essential for the success of the numerical application presented below, where the method is applied to the model potential of Moiseyev, Certain, and Weinhold.[11] The resonances of Moiseyev et al. were obtained along with several others.

In this study we employ the second-order equation

$$y''(x) + \frac{2\mu}{\hbar^2}[\epsilon - q(x)]y(x) = 0. \tag{1}$$

For simplicity we will only consider one equation here. Extensions to the case of coupled equations are easily incorporated in the present formulation, but this will be reported elsewhere. Putting $x \to \eta x$, where η is a complex scale factor with $0 \leqslant \arg \eta < \pi/4$, we obtain the transformed equation,

$$y_\eta''(x) + \frac{2\mu \eta^2}{\hbar^2}[\epsilon(\eta) - q_\eta(x)]y_\eta(x) = 0. \tag{2}$$

In order to emphasize the η dependence, we will write Eq. (2) as a differential equation with the real variable x belonging to the interval $(-\infty, +\infty)$ and the parametric dependence on η indicated by a suffix. We assume that η above is consistent with

$$\lim_{x \to \pm \infty} q_\eta(x) = q_\eta(\pm \infty) = \text{const} < \infty. \tag{3}$$

In terms of the logarithmic derivative

$$\frac{y_\eta'(x)}{y_\eta(x)} = \frac{i\eta}{\hbar} z_\eta(x) ,$$ (4)

we obtain the complex-rotated analog of the Riccati equation

$$\frac{\hbar}{i\eta} z_\eta'(x) = 2\mu[\epsilon(\eta) - q_\eta(x)] - z_\eta^2(x) .$$ (5)

Since we are dealing with the interval $(-\infty, +\infty)$, the condition for an eigenvalue or resonance of Eqs. (1) and (2) is equivalent to finding an energy for which the solution χ is a square integrable at both endpoints. Separating out the even and odd parts of z_η with respect to the coupling constant $\hbar/i\eta$, i.e., $z_\eta = z_\eta^e + z_\eta^o$, one finds that χ may be expressed as

$$\chi = \frac{1}{[z_\eta^e(x)]^{1/2}} \exp\left(\frac{i\eta}{\hbar} \int^x z_\eta^e(s) ds\right) .$$ (6)

Assuming that we have chosen the root $\{2\mu[\epsilon(\eta) - q_\eta(\pm\infty)]\}^{1/2} = k$, $\mathrm{Im}(\eta k) > 0$, we realize that the square-integrable solution should have the following asymptotic forms

$$\chi(x) \simeq \begin{cases} \exp\left(+\frac{i\eta}{\hbar} kx\right), & x \to +\infty \\ \exp\left(-\frac{i\eta}{\hbar} kx\right), & x \to -\infty . \end{cases}$$ (7)
(8)

We now proceed as previously done in the unrotated case by choosing initial value solutions ϕ and ψ as

$$\phi(0) = \sin\alpha, \quad \psi(0) = \cos\alpha,$$
$$\phi'(0) = -\cos\alpha, \quad \psi'(0) = \sin\alpha .$$ (9)

For a given energy ϵ we would combine ϕ and ψ such that $\chi^+ = \phi + m^+\psi$ becomes the square-integrable solution at $+\infty$ and $\chi^- = \phi + m^-\psi$ becomes the one at $-\infty$. Resonance occurs when

$$m^+ - m^- = 0 ,$$ (10)

or in terms of logarithmic derivatives when

$$z_\eta^+(0) - z_\eta^-(0) = 0 ,$$ (11)

where $z_\eta^\pm(0)$ is obtained from (5) via the conditions [see Eqs. (7) and (8)]

$$\lim_{x\to\pm\infty} z_\eta^\pm(x) = \pm k .$$ (12)

As can be seen from Ref. 12 the quantization condition [Eqs. (10) and (11)] is equivalent to finding the poles of the scattering matrix S, or the Green's function, which for $\alpha = \pi/2$ can be written as

$$(m^+ - m^-)^{-1} = \frac{\hbar}{i\eta} [z_\eta^+(0) - z_\eta^-(0)]^{-1} .$$ (13)

Formula (13) is of particular importance in generalizing the present approach to the case of coupled equations.

As a numerical test of the method we used the model potential previously studied by Moiseyev et al.,[11]

$$V(x) = (\tfrac{1}{2} x^2 - J) e^{-\lambda x^2} + J, \quad J = 0.8, \quad \lambda = 0.1 .$$ (14)

The potential is shown in Fig. 1 with its only bound state and its lowest-lying resonances.

To locate the resonances the Hamiltonian is first complex-rotated so as to "open up" the complex energy plane sufficiently, i.e., making the solutions square integrable. The outgoing wave functions are now approximated by the asymptotic forms [Eqs. (7) and (8)] at sufficiently large absolute x values. The corresponding logarithmic derivatives are then propagated to a matching point by numerical integration of the complex-rotated Riccati equation (5). This integration makes use of the log-derivative method due to Johnson,[13] here modified to include the effects of the complex scaling of the coordinates. To efficiently locate the poles of the Green's function, the Newton-Raphson method was employed in the search for the zeros of $|z_\eta^+ - z_\eta^-|$ in the complex energy plane.

Moiseyev et al. gives one of the resonance eigenvalues as

$$E_r - \frac{i}{2} \Gamma = 2.124 - \frac{i}{2} (0.037) .$$ (15)

This value is obtained by investigating the variation of the eigenvalue as a function of the rotation angle. Our calculation predicts the position as

$$E_r - \frac{i}{2} \Gamma = 2.1272 - \frac{i}{2} (0.030 89) .$$ (16)

Our eigenvalues are, furthermore, stable with respect to a variation of the rotation angle, as
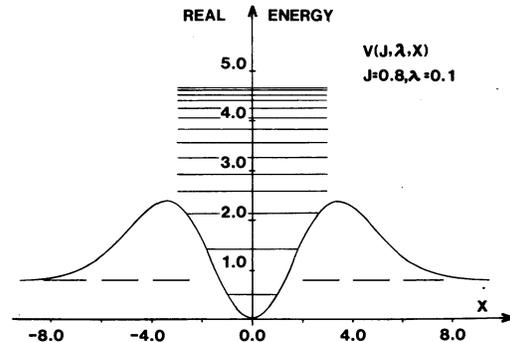
FIG. 1. The test potential was taken from Ref. 11. The calculated bound state and the resonances are indicated with full horizontal lines at their real resonance energies. The asymptotic limit of the potential [$V(\pm\infty)$ $= 0.8$] is indicated with a dashed line.
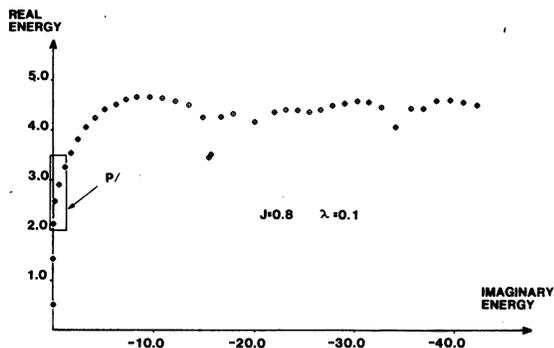
FIG. 2. The calculated resonance positions displayed in the complex energy plane. The rectangle indicated with $P/$ indicates the region where the denominator of the S matrix is displayed in Fig. 3.

FIG. 3. The quantization condition is equivalent of finding the poles of the S matrix or the Green's function which are the same as the poles of $(m^+ - m^-)^{-1}$. $|m^+ - m^-|^{-1}$ is displayed in this figure. The region in the complex plane is indicated as the rectangle $P/$ in Fig. 2.

long as the step size in the integration is kept small enough and the rotation angle is large enough to uncover the pole.

The search for resonances was continued far out in the complex energy plane and Fig. 2 shows the resonance positions. To show the analytic structure of the Green's function, a three-dimensional plot was made (Fig. 3). The peaks correspond to the locations of the resonances, although the fact that the number of points plotted is limited due to our present plotting facilities, makes the peaks lose their actual polelike appearance. Based on the numerical results displayed in Fig. 2, it seems natural to define a complex threshold at a real energy well above the barrier maximum. By this we mean that there exists a real, well-defined, finite energy $E_{thresh} = Re(\epsilon_{thresh})$ such that for all resonance energies ϵ_{res}, we will have

$$Re(\epsilon_{res}) \leq E_{thresh} < +\infty .\qquad(17)$$

As a consequence of this definition it is now possible to partition the resonance spectrum into essentially two classes; the primary and the secondary class. The primary class embodies all resonances with imaginary parts $< Im(\epsilon_{thresh})$, and the secondary class is the complementary set. One would expect the primary resonance to correspond to more or less pronounced peaks in the velocity dependence of the cross section, while the secondary resonances probably accounts for background effects in the framework of potential scattering.

Some immediate implications following from this model study are as follows:

(1) The first implication is the possibility of studying barrier penetration and predissociation phenomena in diatomic molecules, compare for instance Ref. 9, which actually is the original motivation for this work.

(2) The accuracy of a particular Siegert solution, as indicated by its θ stability, implies the possibility of constructing an efficient orbital generator with accurate continuum properties.

(3) The extension to a set of coupled equations is straightforward[14] and is necessary for a more thorough understanding of predissociations in the diabatic framework.

(4) Since the Hartree-Fock equations consist of a set of coupled integrodifferential equations, previous extensions allow for a numerical technique for solving the rotated analog of these equations in the complex plane.

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