Resonance widths and positions of nondilation-analytical potential by the complex-coordinate method

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For nondilation analytic potentials the applicability of the complex coordinate method (CCM) depends on the representation. In particular, it was shown by Colbert, Mashorfer, and Certain that the CCM fails for the Natanzon potential. Analytic expressions for the resonances for this problem were given by Ginocchio and by Alhassid, Iachello, and Levine. It is shown here that the resonances can be obtained by an analytic transformation rather than analytic dilation of the potential.

Resonances are associated with the poles of the resolvent $(E-H)^{-1}$ obtained by analyticaly continuing the resolvent into the lower half of the complex energy plane. One way to carry out the analytical continuation is by using a dilation transformation, $r \rightarrow re^{i\theta}$. The dilation transformation can be presented by the similarity transformation, $\hat{S}\hat{H}\hat{S}^{-1}$, where $\hat{S}$ is the complex scaling operator. For example, in one-dimensional (1D) model systems

$$\hat{S}=\exp\left[\frac{i\theta}{2}(x\hat{p}+\hat{p}x)\right]=e^{\hat{a}}=1+\hat{a}+\frac{(\hat{a})^2}{2}+\cdots .$$

Therefore, the dilation transformation is well defined if the potential is an analytical function for which all the high-order derivatives are defined and if the asymptotic behavior at infinity is not drastically altered. For example, piecewise potentials are not dilation analytic at the matching points where the first-order derivatives are not defined.

The Coulomb interaction belongs to the class of potentials known as dilation analytic potentials. However, the Coulombic electron-nucleus potential interaction term is *not* dilation analytic within the framework of the Born-Oppenheimer approximation (if only the electronic coordinates are scaled). When the nucleii are not at the origin the scaled potential has branch cuts, and therefore the Born-Oppenheimer Hamiltonian is not dilation analytic.

Another possibility is a potential $V(X)$, which is singular at a complex point $X_0=\alpha\exp(i\beta)$. Solutions with two different asymptotical behaviors can be obtained. One type of solution is obtained by carrying out the dilation transformation with $\theta<\beta$ (usually this is considered as the physical solution) whereas, the second type of solution is obtained for $\theta>\beta$. It may occur that a resonance state becomes a square-integrable function only when $\theta>\beta$. In such a case the dilation transformation as presented here is not applicable.

The Natanzon model Hamiltonian is given by[1–4]

$$\left[-\frac{d^2}{dx^2}+v(x)\right]\psi=\epsilon\psi , \quad (1)$$

where

$$v(x)=-\lambda^2\nu(\nu+1)(1-y^2)+(1-y^2)(1-\lambda^2)\times[5(1-\lambda^2)y^4-(7-\lambda^2)y^2+2]/4 , \quad (2)$$

$$x=\frac{1}{2\lambda^2}\left[\ln\frac{1+y}{1-y}+ic\ln\left[\frac{i+cy}{i-cy}\right]\right]=\mathrm{Re}(x) , \quad (3)$$

$$c=(\lambda^2-1)^{1/2} , \quad (4)$$

and λ,ν are dimensionless parameters describing the shape and number of bound states.

Here, $-\infty\leq x\leq\infty$ as $-1\leq y\leq 1$, and in the potential surface there are four singularities at $y=\pm 1$ and $y=\pm i/c$. For the specific values of λ and ν (for example, for the values of $\lambda=26$, $\nu=5.5$) the potential $V(x)$ supports (six) bound states and resonances which result from the tunneling through the two symmetric potential barriers. The resonances are associated with complex eigenvalues $\epsilon=E-i/2\Gamma$, where E is the position and Γ is the width. The resonance eigenfunctions diverge asymptotically but upon scaling the coordinate by

$$x\rightarrow x\exp(i\alpha) , \quad (5)$$

then

$$\psi(xe^{i\alpha})\rightarrow 0 \text{ as } x\rightarrow\pm\infty . \quad (6)$$

As pointed out by Certain and co-workers[4] the condition for a square-integrable resonance function is that

$$\alpha>\phi,\quad \phi=\tfrac{1}{2}\tan^{-1}(\Gamma/2E) , \quad (7)$$

where ϕ is beyond the critical angle $\phi_c=\tan^{-1}(1/c)$ at which the singularity occurs. Therefore, the complex eigenvalues obtained for $\alpha>\phi_c$ do not have the characteristic resonance asymptotical behavior of a purely outgoing plane wave. In order to avoid singularity points and to obtain the resonance complex eigenvalues by bound-state techniques, one can use the Simon exterior scaling procedure,[5] which can be numerically applied in our case,[6] or, as it will be shown here, to choose another set of coordinates.

The transformation of the variable used by Ginocchio,[2]

$$z \equiv \cos\theta = \lambda y / [1+(\lambda^2-1)y^2]^{1/2} , \quad (8)$$

reduces the original Schrödinger equation for the Natanzon potential to the Gegenbauer equation (see Ref. 2):

$$\left[-\frac{d^2}{d\theta^2} + (a+\mu+\tfrac{1}{2})^2 - \left[\frac{\mu^2-\frac{1}{4}}{\sin^2\theta} \right] \right] f(\cos\theta) = 0 , \quad (9)$$

where

$$\mu = (-\epsilon)^{1/2}/\lambda^2 , \quad (10)$$

$$a = [\tfrac{1}{4}+\mu^2(1-\lambda^2)+\nu(\nu+1)]^{1/2} - \mu - \tfrac{1}{2} , \quad (11)$$

and

$$\psi = \left[\frac{\lambda^2+(1-\lambda^2)\cos^2\theta}{\sin^2\theta} \right]^{1/4} f(\cos\theta) . \quad (12)$$

In this step of the calculations the complex coordinate method is used: We make the following transformation:

$$\theta \to \theta + i\alpha \equiv \tilde{\theta} \quad (13)$$

and assume that under this transformation the resonance states become square integrable. (Note that here translation rather than dilation is used because of the boundary conditions that $\mathrm{Re}\theta$ varies from 0 to π.)

The Gegenbauer function $f(\cos\theta)$ is square integrable if

$$a = 0,1,2,\ldots n , \quad (14)$$

where n is a non-negative integer.

From Eqs. (10) and (11) we get

$$\epsilon = -\lambda^2(\nu+\tfrac{1}{2})^2 + (\lambda^2-2)(n+\tfrac{1}{2})^2 + (2n+1)[\lambda^2(\nu+\tfrac{1}{2})^2+(1-\lambda^2)(n+\tfrac{1}{2})^2]^{1/2} . \quad (15)$$

This is exactly the algebraic form of the eigenenergies obtained by Ginocchio for bound states. However, we get that this expression is valid for resonances as well. Complex eigenvalues,

$$\epsilon = -\lambda^2(\nu+\tfrac{1}{2})^2 + (\lambda^2-2)(n+\tfrac{1}{2})^2 \mp i(2n+1) \,|\, \lambda^2(\nu+\tfrac{1}{2})^2+(1-\lambda^2)(n+\tfrac{1}{2})^2 \,|^{1/2} , \quad (16)$$

are obtained when

$$\lambda(\nu+\tfrac{1}{2})^2+(1-\lambda^2)(n+\tfrac{1}{2})^2 < 0 \quad (17)$$

and

$$n > n_0 ,$$
$$n_0 = \lambda(\nu+\tfrac{1}{2})/(\lambda^2-1)^{1/2} - \tfrac{1}{2} . \quad (18)$$

Since resonances are associated with complex eigenvalues $\epsilon = E - \frac{1}{2}\Gamma$, where

$$E = -\lambda^2(\nu+\tfrac{1}{2})^2 + (\lambda^2-2)(n+\tfrac{1}{2})^2 > 0 , \quad (19)$$

then resonances are obtained for

$$n > n_1 ,$$
$$n_1 = \lambda(\nu+\tfrac{1}{2})/(\lambda^2-2)^{1/2} - \tfrac{1}{2}, \quad (20)$$

whereas virtual states are obtained if

$$n_0 < n < n_1 . \quad (21)$$

For large enough values of λ resonances will be obtained if $n > \nu$. The role of the complex variable θ [see Eq. (13)] in the derivation of the closed-form expressions for the resonance positions and widths can be seen by studying the solution of Eq. (9) given by

$$f(\cos\theta) \sim (1-\cos^2\theta)^{(\mu+1/2)/2} C_n^{(\mu+1/2)}(\cos\theta) . \quad (22)$$

[$C_n^{(\mu+1/2)}$ are the Gegenbauer polynomials which diverge if $\mathrm{Re}(\mu) < -\frac{1}{2}$.] For complex $\tilde{\theta} = \theta + i\alpha$ (where α gets an infinitesimal value) the term in the denominator (if $\mathrm{Re}(\mu) < \frac{1}{2}$, $\sin^2\tilde{\theta}$, does not vanish as $\theta = 0$ or π and f remains a square-integrable function as it is for $\mu > 0$ (i.e., bound states). Note, that if f is a square-integrable function the resonance eigenfunction is also in L_2.

The analytical derivation of Ginocchio for bound states is simply extended for resonances. This is the first example where the complex coordinate method (CCM) is analytically applied to a non-dilation-analytic potential, and the second published analytical derivation of resonance positions and widths by the CCM (for the first published analytical example see Doolen, Ref. 7).

The analytical continuation was carried out by transfer θ to $\theta + i\alpha$ rather than by dilation x to $xe^{i\alpha}$.[8] Such analytical continuation has passed the intrinsic nonanalyticities of the potential (by passing on the right-hand side of the singular points in the complex x plane) and enables us to obtain the resonance widths and positions by the CCM.

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