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Note

Shift of the Coordinate Origin in Calculating Resonances by Dilatation Transformation

Resonant scattering is characterized by the energy E and the width Γ of the resonance. Recently, Simon [1] has shown, on the basis of an important theorem of Baslev and Combes [2], that E and Γ may be associated with the complex eigenvalues

$$W = E - i\Gamma/2, \tag{1}$$

of a certain analytically continued Hamiltonian operator $H_\theta = H(\vec{r}e^{i\theta})$. This operator is obtained from the ordinary self-adjoint Hamiltonian $H(\vec{r}) = T(\vec{r}) + V(\vec{r})$ when the position vectors $\vec{r}$ are rotated upward into the complex coordinate plane:

$$\vec{r} \to \vec{r}e^{i\theta}, \qquad \theta > 0, \quad \text{real.} \tag{2}$$

In this way, E and Γ can be simply obtained by solving a non-Hermitian eigenvalue problem.

A detailed mathematical justification of the dilatation–transformation method is given in [1, 2] for the limited class of so-called dilatation analytic potentials. However, some authors [3–5] have calculated E and Γ successfully for potentials that do not belong to this class.

For example, Yaris *et al.* [5] use the dilatation–transformation method to identify resonances in the cubic anharmonic oscillator

$$H = p_x^2 + x^2/4 - \lambda x^3, \qquad p_x = -id/dx, \quad \lambda > 0. \tag{3}$$

In this case, the eigenvalues W of the rotated Hamiltonian H_θ are computed by way of an expansion in a properly chosen basis set and then solving the truncated eigenvalue equation exactly [4]. Owing to the finite-basis-set approximation, the position of a resonance eigenvalue is not completely independent of θ, as it should be if the eigenvalue equation were exactly solved. What is usually done is to repeat the diagonalization for different values of θ to find that value of θ for which $W(\theta)$ is most nearly stable [5, 6]. The accuracy of the computed resonances is estimated by increasing the size of the truncated basis set. Besides, the rate of convergence of the resonances as a function of the size of the truncated basis set depends on the basis set itself. Therefore, it is of great importance to choose it carefully.

This note will show how to find a good basis set to identify resonances in problems which do not possess a center of inversion. To simplify the discussion the Hamiltonian (3) will be used as an illustrative example.

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Yaris *et al.* [5] used the set of eigenfunctions of $p_x^2 + k^2x^2/4$ in order to diagonalize H and found the best value of k. But since the potential function is not symmetric about $x = 0$, we are allowed to use a shifted harmonic oscillator basis set. This is obtained by means of the following transformation:

$$z = 2^{1/2} a x e^{i\theta} + b, \tag{4}$$

where a, b, θ are real and $\theta > 0$. Obviously, a plays the role of k and has the usual meaning. But the new parameter b takes into account the fact that the potential in (3) does not have a center of inversion (that is to say: the potential is not an even function of the coordinate).

The transformation (4) leads to a new Hamiltonian $H_{ac\theta}$,

$$\begin{aligned} H_{ac\theta} = H(x(z)) = {} & \tfrac{1}{2} a^2 e^{-2i\theta} p_z^2 + a^{-2}(\tfrac{1}{2} e^{2i\theta} - 3\lambda' c e^{3i\theta})\, z^2 - \lambda' a^{-3} e^{3i\theta} z^3 \\ & + a^{-1}(c e^{2i\theta} - 3\lambda' c^2 e^{3i\theta})\, z + \tfrac{1}{2} c^2 e^{2i\theta} - \lambda' c^3 e^{3i\theta}, \end{aligned} \tag{5}$$

where $c = -b/a$ and $\lambda' = 2^{3/2}\lambda$.

The eigenvalues of $H_{ac\theta}$ are obtained by expanding it in a truncated basis set of normalized eigenfunctions $\{\phi_n\}$ of $H_0 = p_z^2 + z^2$ and then solving the matrix eigenvalue equation

$$\{\mathbf{H}_{ac\theta} - W_n(a, c, \theta)\, \mathbf{I}\}\, \mathbf{C}_n = 0, \tag{6}$$

where $\mathbf{H}_{ac\theta}$ and $\mathbf{I}$ are $N \times N$ matrices corresponding to the Hamiltonian and to the identity operator, respectively. $\mathbf{C}_n$ is an N-dimensional row vector.

If the real parameters a and c are properly chosen, the rate of convergence of the eigenvalues W_n as functions of the size N of the basis set increases. This has been proved in the case of real scaling calculations [7]. The aforesaid conclusion also holds when a complex scaling calculation is performed.

It only remains to obtain proper values for a and c. The parameter θ will be determined according to the above-mentioned criterion [5, 6]. Since the exact eigenvalues W_n are not dependent on a and c, it is appropriate to choose those values of a and c that make $W_n(a, c, \theta)$ stable. But this procedure leads to a large amount of computation, a task to be avoided.

Acceptable values for a and c are the stationary points of $\mathscr{E}_n(a, c) = \langle \phi_n | H_{ac0} | \phi_n \rangle$,

$$\mathscr{E}_n(a, c) = (n + \tfrac{1}{2})(\tfrac{1}{2} a^2 + \tfrac{1}{2} a^{-2} - 3a^{-2} c\lambda') + \tfrac{1}{2} c^2 - \lambda' c^3; \tag{7}$$

that is to say, the roots of

$$a^4 - 6\lambda' c - 1 = 0, \tag{8a}$$

$$-3(n + \tfrac{1}{2})\, a^{-2}\lambda' + c - 3\lambda' c^2 = 0. \tag{8b}$$

If $\lambda' = 0$, then $c = 0$. This choice is reasonable since $\mathscr{E}_n(a, c)$ equals $W_n(a, c, \theta)$ when $\theta = 0$ and $N = 1$ (N is the matrix dimension in (6)).

The matrix elements in the expansion of $H_{ac\theta}$ in the chosen basis set $\{\phi_n\}$ are easily shown to be:

$$(\mathbf{H}_{ac\theta})_{ij} = \left\{\left(i+\frac{1}{2}\right)a^{-2}\left(\frac{1}{2}a^4e^{-2i\theta}+\frac{1}{2}e^{2i\theta}-3\lambda' ce^{3i\theta}\right)+\frac{1}{2}c^2e^{2i\theta}-\lambda' c^3e^{3i\theta}\right\}\delta_{i,j}$$
$$+\frac{1}{2}(i+1)^{1/2}(i+2)^{1/2}a^{-2}\left(-\frac{1}{2}a^4e^{-2i\theta}+\frac{1}{2}e^{2i\theta}-3c\lambda' e^{3i\theta}\right)\delta_{i+2,j}$$
$$+\left\{\left(\frac{i+1}{2}\right)^{1/2}a^{-1}(ce^{2i\theta}-3c\lambda' e^{3i\theta})-3\left(\frac{i+1}{2}\right)^{3/2}a^{-3}\lambda' e^{3i\theta}\right\}\delta_{i+1,j}$$
$$-\left\{\frac{(i+1)(i+2)(i+3)}{8}\right\}^{1/2}a^{-3}\lambda' e^{3i\theta}\delta_{i+3,j}. \tag{9}$$

To solve the eigenvalue problem (6), we use a modified LR algorithm [8] after performing a similarity reduction of $\mathbf{H}_{ac\theta}$ to a Hessenberg form [9]. All calculations are performed using the values of a and c that result from (8) when $n=0$. This choice assures the highest convergence rates for the low-lying resonances.

The energies and the widths of the resonances of the model (3) (with $\lambda=0.03$) are shown in Table I, where two different calculations are compared: (i) when a, b are solutions of (8) and (ii) when $a=0.8$ and $b=0$, which correspond to the calculation in Ref. [5] with $k=0.4$. In both cases $\theta=0.2$ is used. The introduction

TABLE I

Resonances in $H=p_x^2+x^2/4-\lambda x^3$ when $\lambda=0.03$

N	n	Re $W_n{}^a$	$-$Im $W_n{}^a$	Re $W_n{}^b$	$-$Im $W_n{}^b$
10	0	0.489196055	9.5×10^{-7}	0.489217619	1.8×10^{-5}
	1	1.422932675	7.6×10^{-5}	1.423124774	3.0×10^{-5}
	2	2.251292943	1.1×10^{-2}	2.249105930	5.5×10^{-3}
	3	2.959113806	0.12	2.919107389	0.14
	4	3.739108908	0.39	3.461815929	0.43
20	0	0.489194714	5.52×10^{-8}	0.489194720	5.70×10^{-8}
	1	1.422922313	4.09×10^{-5}	1.422922404	4.08×10^{-5}
	2	2.250200574	7.43×10^{-3}	2.250203205	7.40×10^{-3}
	3	2.923853339	0.139	2.923358810	0.139
	4	3.619868351	0.462	3.616822098	0.468
30	0	0.489194714	5.54×10^{-8}	0.489194714	5.54×10^{-8}
	1	1.422922458	4.09×10^{-5}	0.422922457	4.09×10^{-5}
	2	2.250199666	7.41×10^{-3}	2.250199673	7.41×10^{-3}
	3	2.923356344	0.139	2.923359372	0.139
	4	3.618976541	0.469	3.618942705	0.469

[a] $a=0.9821258$, $c=0.1367116$, $\theta=0.2$.
[b] $a=0.8$, $c=0$, $\theta=0.2$.

of the parameter b that takes into account the potential symmetry improves the rate of convergence markedly for both the real and imaginary part of the two lowest resonances (see Table I). All the calculations show that the convergence rate depends more strongly on c rather than on a. This confirms the importance of the parameter c.

The results obtained in this note using the simple (though nontrivial) one-dimensional quantum-mechanical model (3) confirm that the introduction of adjustable parameters that change the coordinate origin increases the convergence rates of the eigenvalues of a finite-dimensional vector-space eigenvalue equation like (6) in those cases where there is not a center of inversion. This conclusion applies to many-dimensional models too, as suggested by real scaling calculations performed earlier [7].

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ALEJANDRO M. MESÓN
FRANCISCO M. FERNÁNDEZ
EDUARDO A. CASTRO

INIFTA, División Química Teórica,
Sucursal 4, Casilla de Correo 16,
La Plata 1900, Argentina

ALBERTO MALTZ
RODOLFO RODRIGUEZ

Departamento de Matemáticas,
Facultad de Ciencias Exactas,
UNLP, Casilla de Correo 172,
La Plata 1900, Argentina