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LETTER TO THE EDITOR

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Abstract. A modified version of the least-squares variational technique is proposed to calculate resonance energies and widths with the help of the coordinate-rotation method. A numerical example is given for a model potential.

A narrow scattering resonance is always associated with a long-lived decaying state which behaves physically, in many respects, like a true bound state. By introducing a generalized non-Hermitian scalar product and using the resonance definition of Siegert (1939), Berggren (1968) showed that for finite-range potentials, the bound states and any finite number of proper resonant states could be completed by an appropriately chosen set of continuum states. The physical resemblance between bound states and narrow resonances was specially demonstrated by Gyarmati *et al* (1972), calculating expectation values in Gamow states.

It is desirable, however, to develop approximation techniques for computing resonance energies and widths simultaneously. Recently, Bain *et al* (1974) have applied the Rayleigh–Ritz variational method combined with complex contour integration to Gamow (or Siegert) states. The Rayleigh–Ritz method has also been used by Doolen *et al* (1973, 1974) and by Raju and Doolen (1974) but with the trick of the rotation of the Hamiltonian in the complex coordinate space. These two methods, however, are not based upon an extremum principle, since the functionals applied are only stationary around the complex resonance energy, and the convergence is questionable in the case of large basis sizes.

Here, we propose an alternative variational technique for the calculation of square-integrable eigenfunctions and complex or real eigenvalues of the rotated Hamiltonian. The variational method is the well known least-squares method, extensively applied to non-relativistic bound state (Preuss 1962) and scattering (Ladanyi and Szondy 1971, Read and Soto-Montiel 1973, Schmid and Schwager 1972), as well as relativistic bound state (Ladanyi 1968) and scattering (Ladanyi 1969) problems.

Applying the coordinate-rotation $r \to r\,e^{i\theta}$ to the total Hamiltonian H, we get

$$H = H_0 + V(r) \to H^\theta = e^{-2i\theta} H_0 + V(r\,e^{i\theta}),$$

where H_0 and V are the kinetic- and potential-energy operators, respectively. The complex eigenvalues of H^θ, $W_n = E_n - \frac{1}{2}i\Gamma_n$, with vanishing boundary condition at infinity, can be identified as the resonance poles of the analytically continued S-matrix for the original problem (Lovelace 1964), and are independent of θ for $|\arg W_n| < 2\theta < a$, where a depends on the analyticity domain of the potential V (Aguilar and Combes 1971).

The following eigenvalue equation has to be solved:

$$(H^\theta - W)\psi \equiv L\psi = 0, \qquad (\psi(0) = 0, \psi \underset{r \to \infty}{\to} 0), \tag{1}$$

where L is a linear, but not self-adjoint, operator on the Hilbert space, for W complex. The trial function is

$$\psi' = \sum_{n=1}^{N} a_n \phi_n,$$

where $\phi_1, \phi_2, \ldots, \phi_N$ are elements of a complete set of quadratically integrable basis functions and the coefficients a_n are complex linear variational parameters. Let P^K, $K > N$, be a projection operator $\{(P^K)^2 = P^K, (P^K)^\dagger = P^K\}$, projecting onto an arbitrary K-dimensional subspace of the Hilbert space. Let us define the square of the length of the projection of the vector $L\psi'$ (or the square-error expression of ψ') in the K-dimensional space by

$$\sigma^K(\psi', E, \Gamma) = \langle \psi' L P^K, P^K L\psi' \rangle / \langle \psi', \psi' \rangle, \tag{2}$$

where the denominator means a formal norm of ψ' for the square-error expression. One has $\sigma^K \geq 0$ by construction and the equality holds if ψ' is the exact solution of equation (1), or $L\psi'$ is, accidentally, orthogonal to the subspace defined by P^K. The variational requirement $\delta\sigma^K(\psi') = 0$, for E, Γ fixed, leads to a positive symmetrical $2N \times 2N$ matrix eigenvalue equation, where the lowest eigenvalue $\sigma_0^K(E, \Gamma)$ yields the minimum of $\sigma^K(\psi')$ for E, Γ fixed. The role of the norm $\langle \psi', \psi' \rangle$ in equation (2) is only to exclude the trivial solution $\psi' \equiv 0$, of equation (1).

We are now in a position to calculate the least-squares approximation of the resonance parameters E_n and Γ_n by minimizing $\sigma_0^K(E, \Gamma)$ according to the conditions

$$\partial\sigma_0^K(E, \Gamma)/\partial E = 0, \tag{3a}$$

and

$$\partial\sigma_0^K(E, \Gamma)/\partial\Gamma = 0. \tag{3b}$$

Although the energy W_n is initially unknown, an estimate of the resonance position as starting value for equations (3) can be made, for instance, by the stabilization method (Hazi and Taylor 1970).

Since $\sigma_0^K(E, \Gamma)$ is obtained by varying only the linear parameters in ψ', an optimization is needed with respect to the nonlinear scale parameters involved, in order to get the best convergence.

Here we note that our procedure, though conceptually different, reduces to that of Froelich and Brändas (1975) by choosing $\theta = \Gamma = 0$, $P^K = 1$ and $\langle \psi', \psi' \rangle = \langle \psi', \psi' \rangle = 1$.

As an illustrative example, we have computed the resonance parameters E and Γ for the potential $V(r) = 7 \cdot 5r^2 e^{-r}$, where the exact values were known (Bain *et al* 1974). Table 1 shows the resonance energy E and width Γ with different values of K, $K > N$, as the number N of the basis functions increases. The calculation was carried out by using Slater-type functions:

$$\phi_n = r^n e^{-\alpha r}, \qquad (n = 1, 2, \ldots, N),$$

Table 1. Calculated resonance parameters† for the model potential; $d = K - N$.

N	Energy (au)		Width (10^{-2} au)	
	$d = 3$	$d = 5$	$d = 3$	$d = 5$
4	3·3816	3·3898	2·0538	2·1116
6	3·4032	3·4100	2·5670	2·5612
8	3·4283	3·4271	2·5563	2·5550
10	3·4266	3·4264	2·5545	2·5548
12	3·4264	3·4264	2·5548	2·5549

† Exact values: $E = 3·42639$ au, $\Gamma = 2·5549 \times 10^{-2}$ au.

and

$$P^K = \sum_{j=1}^{K} \chi_j \rangle\langle \chi_j ,$$

with

$$\chi_j = \left(\frac{(2\beta)^{2j+1}}{(2j)!} \right)^{1/2} r^j e^{-\beta r}, \qquad (j = 1, 2, \ldots , K),$$

where the nonlinear parameters α and β were taken to be 3·5. The rotation angle θ was 0·5 rad. Several calculations, not presented here, show that the final results do not depend sensitively on the variation of α, β and θ for large basis sizes, $N \geqslant 10$.

Finally, it should be emphasized that, in the case of interacting many-body systems, the projection operator P^K, $N < K < \infty$, included in equation (2) does simplify the calculation of the necessary matrix elements.

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