Variational study of a continuum crossing model

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A model S-wave crossing of a bound state into the continuum is investigated using nonlinear variational calculations performed with the exact wave function and a trial function which has incorrect asymptotic behavior. The variational estimates of the energy-branch structure become less accurate near threshold, as expected, but the calculations indicate a sequence of branches which are followed in order to obtain estimates of the energy and width of a decaying-state resonance above threshold.

I. INTRODUCTION

There has been much interest recently in L^2 approaches for estimating the energies and widths of resonances.[1] This work is concerned with the accuracy of an L^2 approach for a near-threshold resonance, and in particular the crossing of an ordinary bound state below threshold into the continuum by means of adjustable parameters contained in the potential energy.[2] Variational calculations with a limited basis may fail to reproduce the exact crossing behavior, which is sensitive to the long-range part of the wave function. Moreover, it is expected that limited-basis calculations including nonlinear variations of orbital exponents, for example, may include spurious stationary solutions in addition to the one which best approximates the actual resonance. In order to gain some additional insight to this problem, we have carried out the detailed numerical solution of a relatively simple S-wave crossing of the ground state of the Schrödinger equation $(H-E)\psi=0$ for the Hamiltonian

$$H=-\frac{1}{2}\frac{d^2}{dx^2}+\delta(x-1)+v(x) \tag{1}$$

which includes an intermediate-range δ-function barrier plus a short-range square well,

$$v(x)=\begin{cases}2\lambda, & 0<x<1\\ 0, & x>1\\ \infty, & x\leq 0,\end{cases} \tag{2}$$

where the parameter λ controls the well depth.

II. EXACT SOLUTION

Elementary procedures give the exact bound-state wave function

$$\psi=\begin{cases}A\sin(\alpha x), & 0\leq x\leq 1\\ \exp(-\eta x), & x\geq 1\end{cases} \tag{3}$$

with A, α, and η determined from matching and the cusp condition $\eta+2\alpha\cot(\alpha)=0$ at $x=1$. From the point of view of variational theory, the energy eigenvalues correspond to stationary values of

$$E=(\psi,H\psi)/(\psi,\psi) \tag{4}$$

in which the long-range exponent η is treated as a single variational parameter, and the matrix element of an operator F is defined by

$$(\psi,F\psi)=\int_0^\infty \psi(F\psi)dx\,. \tag{5}$$

In general the stationary solutions include complex orbital exponents $\eta=r\pm im$ and energies $E=E_r\pm\frac{1}{2}i\Gamma$ with m and Γ positive or zero. Following standard convention, we shall distinguish between solutions for bound states ($E_r<0$, $\Gamma=0$, $r>0$, $m=0$), virtual states ($E_r<0$, $\Gamma=0$, $r<0$, $m=0$), and decaying states ($E_r-\frac{1}{2}i\Gamma$, $\eta=r-im$) that are associated with resonance behavior on the real-energy axis. In the variational calculations, these latter states are found by suitable analytic continuation of (4) with complex orbitals.

The exact results for the nodeless ground state are shown in Fig. 1. For convenience the energies are given as $\epsilon=2E=\epsilon_r-i\Gamma$. The continuum threshold lies at zero energy. Branch A is the bound state and corresponds to a minimum in the real part of the energy as a function of r. A is tangent to the continuum edge at $\lambda_a=-5.239$, where $r=0$. B labels the virtual state, which has a real energy corresponding to a minimum with respect to r. A third, unphysical solution is C, which occurs as a real-energy maximum in the variational calculations. The confluence of B and C at $\lambda_b=-4.975$ marks a $\frac{1}{2}$-power branch point in the energy as a function of λ, illustrated by the width in Fig. 1(b) for the decaying-state branch D. In contrast, the real-energy part of D in Fig. 1(a) shows a nearly linear increase with λ. Analysis of the variational energy formula shows that the leading-order behavior near the confluence at λ_b is

$$E=AZ^{-1}+B+CZ\,, \tag{6}$$

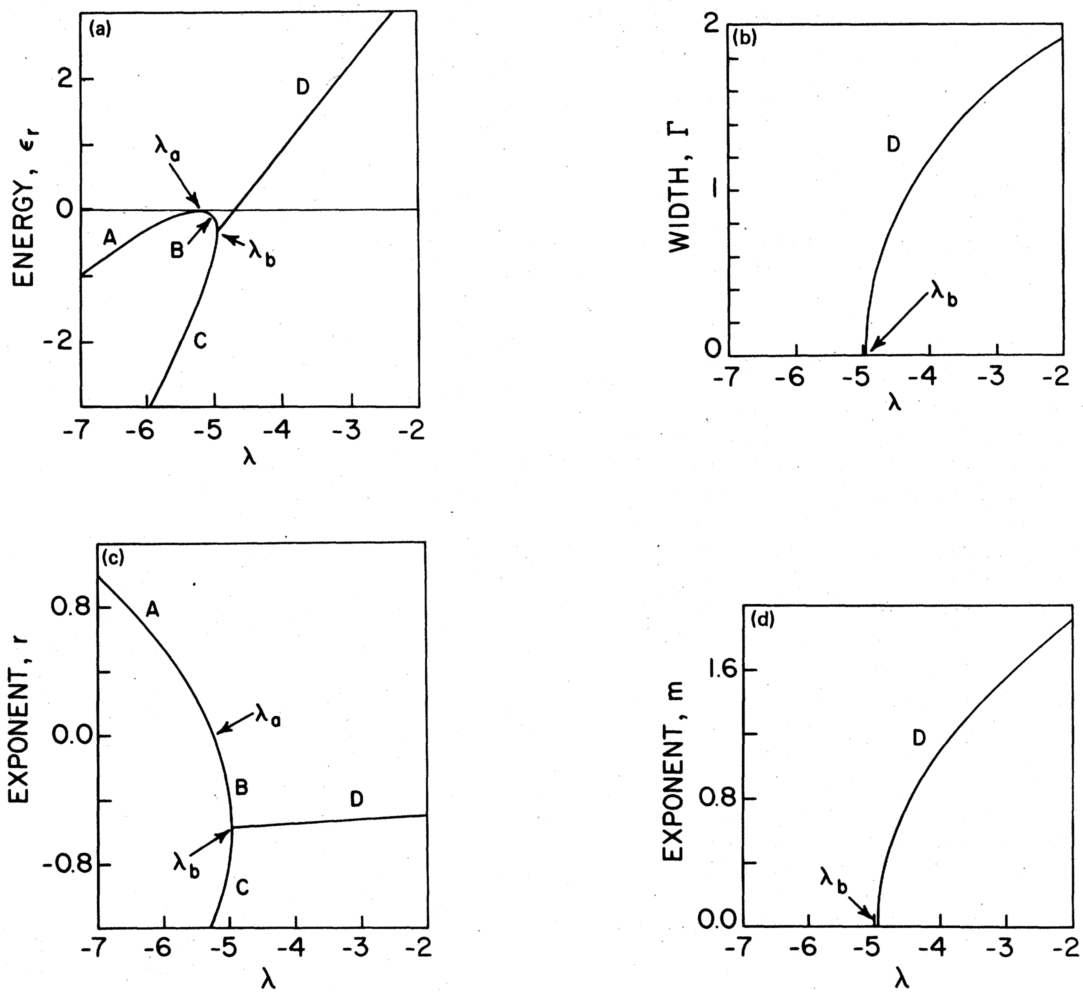

FIG. 1. (a)–(d) Branch structure for the exact ground-state solution of the continuum crossing model (1), shown as a continuous function of the well-depth parameter λ.

where A, B, and C are functions of λ only, and $Z \equiv \eta - \eta_b$ is a variational parameter. The stationary condition $\delta E = 0$ gives $Z^2 = A/C$, and hence

$$E = B \pm (4AC)^{1/2} . \qquad (7)$$

The $\frac{1}{2}$-power energy branch is due to a simple zero $A \propto \lambda - \lambda_b$. The singularity Z^{-1} in (6) is due to a zero in the overlap integral (ψ, ψ) in (4). Linearity of the real part of the energy and orbital exponent when $\lambda > \lambda_b$ in Figs. 1(a) and 1(c) is associated with higher-order terms in the energy than are included in (6), and is found to be linked to the leading-order formula $\lambda \simeq \lambda_b + \alpha Z^2 + \beta Z^3$ with real constants α and β when $\lambda < \lambda_b$.

III. VARIATIONAL ESTIMATES WITH A NONEXACT ψ

We have repeated the variational calculations for the ground-state continuum crossing using an incomplete basis represented by the trial function

$$\psi = \begin{cases} A \sin(\alpha x), & 0 \leq x \leq 1 \\ x \exp(-\eta x), & x > 1 . \end{cases} \qquad (8)$$

The purpose of choosing this incorrect asymptotic form of the wave function is to give a concrete example of additional complexity that is consequently introduced into the branch structure for the continuum crossing. It is assumed that the cusp condition $\eta + 1 + \alpha \cot(\alpha) = 0$ is satisfied at $x = 1$, so that the variational energy is a function of only the asymptotic orbital exponent η.

The results are shown in Figs. 2(a)–2(d), which may be compared, respectively, with the exact solutions in Figs. 1(a)–1(d). Here we find a more complicated structure, although curves A, B, C, and D represent approximate versions of the exact ones. Branches B and D are now complex energy

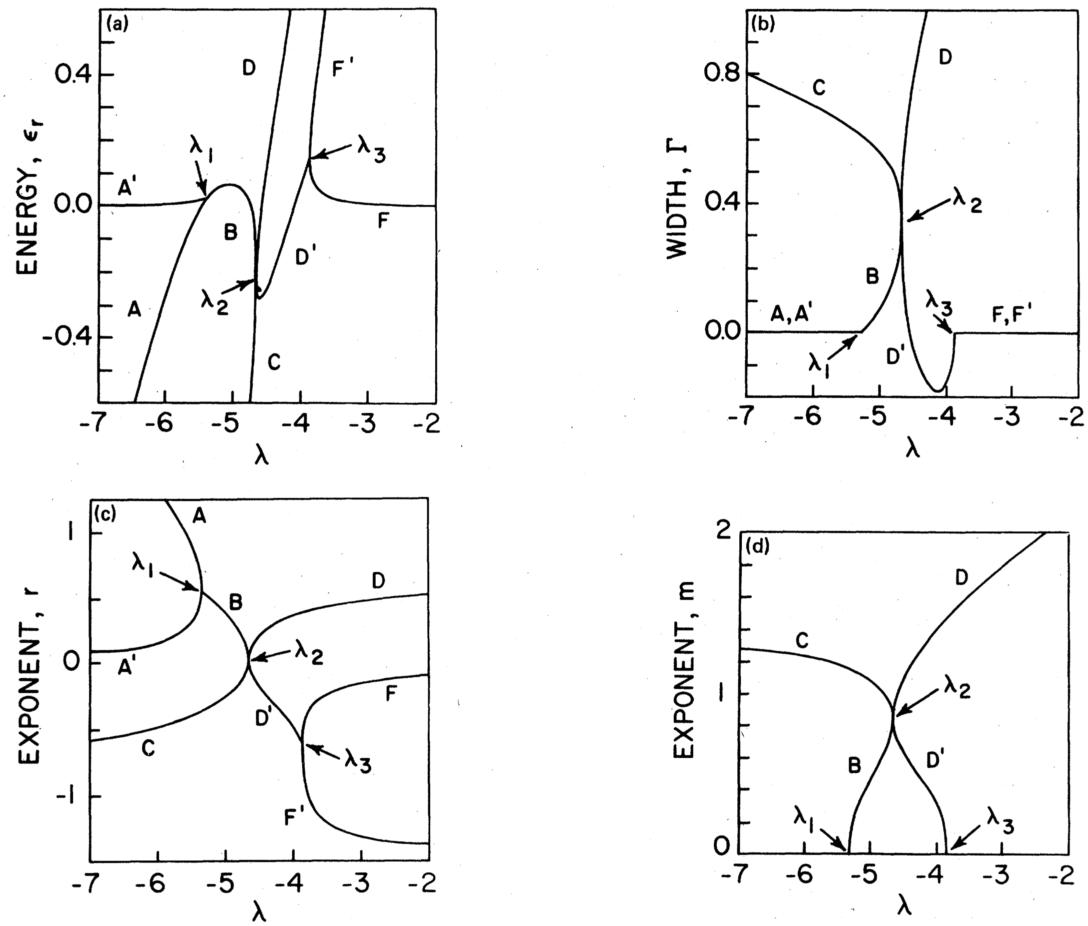

FIG. 2. (a)–(d) Variational estimates of the ground-state continuum crossing branch structure obtained from the trial wave function (8).

solutions, however, and two new branches labeled A' and F in Fig. 2(a) represent variational estimates of the continuum edge. Real-energy branches A and F occur as minima with respect to r, while A' and F' occur as maxima in the variational calculation. The curve F is the one that is usually associated with the collapse of variational calculations in the continuum since it is the lowest energy solution in this λ regime and has a very diffuse wave function [see Fig. 2(c)].

The points λ_1 and λ_3 mark the confluence of real-energy minima and maxima branches. The energy has a $\frac{3}{2}$-power branch point at $\lambda = \lambda_1$, much like the singularities found in nonlinear variational calculations with atoms.[2] The basic structure is illustrated with a cubic representation of the variational energy near a singular point λ_c:

$$E = A + BZ + CZ^3, \qquad (9)$$

where A, B, and C are again functions of only λ, and $Z = \eta - \eta_c$. The stationary condition gives $Z^2 = -B/3C$, and hence

$$E = A \pm (4B^3/27C)^{1/2}. \qquad (10)$$

The confluence of the two branches A and A' at λ_1 is described by (10) when B has a simple zero, $B \propto \lambda - \lambda_1$. The resulting $\frac{3}{2}$-power branch singularity in the energy was not part of the exact structure in Fig. 1(a), and offers an example of the type of spurious behavior that can arise. λ_2 and λ_3 correspond to $\frac{1}{2}$-power branch points in Fig. 2(a). The singularity at λ_2 is similar to the one at λ_b in Fig. 1(a), except that now the variational parameter η is complex.

The interesting point illustrated by these calculations is that the branching route $A \rightarrow B \rightarrow D$ continues to represent the exact continuum crossing route *bound state* $\rightarrow$ *virtual state* $\rightarrow$ *decaying state*. It would be more difficult to identify the physical decaying-state energy in calculations performed at only a single value of λ. The largest differences between the estimated and exact resonance parameters occurs near threshold, as expected. The estimated width differs from the exact one by less than 1% when $\lambda > -2$, however, where threshold effects are smaller. An extended profile of the width for higher λ is given in Fig. 3.

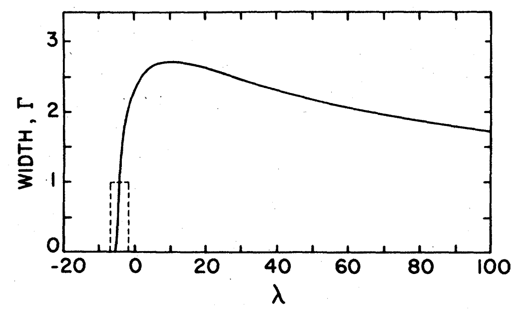

FIG. 3. Variational estimate of the width of the decaying state resonance. The smaller rectangular region is shown separately in Fig. 2(b), including only branches *B* and *D*.

IV. SUMMARY

The present calculations of a simple model problem have illustrated the necessarily increased complexity of the energy-branch structure in variational estimates of a decaying state near threshold. An important result was the identification of a "road map" for the variational estimates which gave a reasonable approximation of the exact crossing structure. Although increasing the number of variational parameters in the trial function generally improves the bound-state energies, the present results suggest that additional complexity of the branching structure near threshold might also develop. Although the problem of multiple energy branches seems to be avoided in linear variational approaches with a scaled Hamiltonian,[1] where spurious eigenvalues move far off the real axis as the basis size is increased, they cannot be ignored in nonlinear approaches such as a multiconfigurational treatment which includes a variable orbital exponent for the decay channel.[2]

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