A class of exactly solvable models to illustrate supersymmetry and test approximation methods in quantum mechanics

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We obtain analytical expressions for the eigenvalues and eigenstates of a family of exponential-type potential wells. The supersymmetry formalism applied to quantum mechanics is summarized and illustrated by producing from this family of potentials another class of exact solutions made of their isospectral partners. A subset of the supersymmetric partners provides a class of exactly solvable double well potentials. The exact solutions of these potentials are used to test the robustness and accuracy of different approximation methods. We determine the ground state through a variational method applied to a set of trial functions and the entire spectrum using the WKB, JWKB, and its supersymmetric extension formulas. We comment on the importance of the Maslov index and on the range of validity of these semiclassical quantization approaches. © *2011 American Association of Physics Teachers.*

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I. INTRODUCTION

Analytically solvable models in quantum mechanics are of much interest because they allow the abstract theoretical framework to be illustrated by concrete examples. For instance, the square well potential is convenient for introducing the notion of reflection and transmission coefficients for the scattering states with a minimum of calculations, yielding some astonishing results such as the total quantum reflection of a low incident energy particle interacting with a potential well. Besides the square potential, there are not many scattering one-dimensional potentials that are discussed in quantum mechanics textbooks. Reference 1 gives the interesting example of the step potential $U(x)=U_0/(1+e^{\alpha x})$, for which one has to deal with subtle asymptotic conditions at infinity to solve the scattering problem.

Interestingly, once an analytical solution is known, supersymmetry techniques applied to quantum mechanics provide a whole family of analytical solutions having closely related properties. Analytically solvable models provide a way for comparing approximate methods to exact solutions and can be used to model more complex situations.

In this article, we first investigate a family of one-dimensional exponential-type potential wells. In contrast to square well potentials, these potentials are characterized by two parameters—the depth of the potential U_0 and the typical length of variation α^{-1} of the potential (see Fig. 1). We solve the scattering problem analytically and determine the bound states. This family of potentials provides an interesting example of the role of parity symmetry and the importance of boundary conditions on the existence and the number of bound states.

The second part of the article is devoted to the use of the supersymmetry formalism for exponential potential wells[2,3] and a new class of exactly solvable double well potentials.

The third part explores the robustness and accuracy of approximation methods in quantum mechanics. We compare the exact energy of the ground state for exponential potentials with approximate results based on variational calculations. We give examples of the importance of the appropriate set of trial functions to obtain an accurate estimate of the ground state along with the limitations of this method. The exact bound spectrum of the potential wells is also compared with the predictions of different semiclassical quantization formulas. We recover general conclusions on the relative range of validity of these different approaches.

II. EXPONENTIAL POTENTIALS

We first solve for the eigenstates for potentials $U_{\mathrm{I}}(x)$ defined for $x>0$ with a sharp wall at $x=0$ and then for even potentials $U_{\mathrm{II}}(x)$ defined on the entire real axis with only soft walls. We have

$$U_{\mathrm{I}}(x)=\begin{cases}-U_0e^{-\alpha x} & (x>0)\\ \infty & (x<0)\end{cases} \tag{1}$$

and

$$U_{\mathrm{II}}=-U_0e^{-\alpha|x|}, \tag{2}$$

with $\alpha>0$. We set $U_0>0$ because we are considering potential wells.[5] The potentials $U_{\mathrm{I}}(x)$ and $U_{\mathrm{II}}(x)$ are represented in Fig. 1.

The determination of the motion of a particle of mass m that experiences $U_{\mathrm{I}}(x)$ or $U_{\mathrm{II}}(x)$ requires the knowledge of the stationary states, which are solutions of the time-independent Schrödinger equation. If we introduce the dimensionless variable $X=\alpha x$ and the dimensionless parameters $a=[8mU_0/(\hbar^2\alpha^2)]^{1/2}$ and $b=[8m(-E)/(\hbar^2\alpha^2)]^{1/2}$, we can express the time-independent Schrödinger equation in the form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}X^2}+\frac{1}{4}[a^2e^{-X}-b^2]\psi(X)=0. \tag{3}$$

By making the change of variable $y=ae^{-X/2}$, Eq. (3) takes the form of the second-order differential equation satisfied by the Bessel functions,

$$y^2\frac{\mathrm{d}^2\psi}{\mathrm{d}y^2}+y\frac{\mathrm{d}\psi}{\mathrm{d}y}+[y^2-b^2]\psi(y)=0. \tag{4}$$

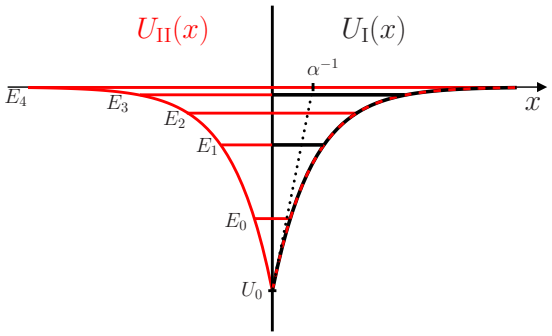

Fig. 1. (Color online) Potentials $U_{II}(x)$ and $U_I(x)$ of depth U_0 and characteristic length α^{-1}. $U_{II}(x)$ is plotted with five bound states ($a=8.48$) with energies $E_4>E_3>E_2>E_1>E_0$, and $U_I(x)$ is represented for the same parameters. This latter potential accommodates only two bound states with energies E_3 and E_1.

A. The bound energies and states of $U_I(x)$

The energy of the bound states of the potential well $U_I(x)$ is found for energy $E<0$ (b is real and positive). In this case, the solution of Eq. (3) takes the form

$$\psi(X\geq 0)=A_1^+J_b(ae^{-X/2})+A_2^+J_{-b}(ae^{-X/2}), \tag{5}$$

where J_b are the Bessel functions of the first kind. The spectrum is determined by the boundary conditions, $\psi(0)=0$ and $\psi(x\to\infty)=0$, and we obtain

$$A_1^+J_b(a)+A_2^+J_{-b}(a)=0, \tag{6}$$

$$[A_1^+J_b(y\to 0)+A_2^+J_{-b}(y\to 0)]\to 0. \tag{7}$$

We have $J_\nu(y\to 0)\propto y^\nu$. Because $b>0$, the divergence of $J_{-b}(y)$ when $y\to 0$ requires that $A_2^+=0$ to satisfy Eq. (7). The discrete spectrum of energy $\{E_n\}$ is therefore obtained from Eq. (6) and involves the zeros $\{b_n\}$ of the Bessel function for fixed values of U_0 and α,

$$J_{b_n}(a)=0. \tag{8}$$

The number of bound states is thus dictated by the value of the parameter a. The ground state energy is $E_0=-U_0b_0^2/a^2$. The wave function associated with the eigenenergy E_n is

$$\psi_n(x)=\mathcal{N}_nJ_{b_n}(ae^{-\alpha x/2}), \tag{9}$$

where $\mathcal{N}_n$ is a normalization factor. If $a<a_c\simeq 2.405$, there is no value of b that satisfies Eq. (8), meaning that the potential U_I does not have a bound state. The sharp wall of the potential at $x=0$ rules out the application of the theorem, according to which there is always at least a bound state for a one-dimensional potential.[6,7] The analysis of the bound states of $U_{II}(x)$ enables a simple interpretation of the nonexistence of a bound state for $U_I(x)$ when $a<a_c$.

B. The bound energies and states of $U_{II}(x)$

The general form of the solution of the stationary Schrödinger equation for the potential $U_{II}(x)$ is

$$\psi(X\geq 0)=A_1^+J_b(ae^{-X/2})+A_2^+J_{-b}(ae^{-X/2}), \tag{10a}$$

$$\psi(X\leq 0)=A_1^-J_b(ae^{X/2})+A_2^-J_{-b}(ae^{X/2}). \tag{10b}$$

$U_{II}(x)$ is even and thus commutes with the parity operator. As a result, the eigenfunctions have a well-defined parity. The determination of the bound states is made by searching for solutions such that $\psi(x\to\pm\infty)=0$, which implies that $A_2^+=A_2^-=0$, with the extra conditions $\psi(0)=0$ for the odd solutions and $\psi'(0)=0$ for the even solutions. For a given value of a, the corresponding discrete spectrum is given by the zeros $\{b_n\}$ of the Bessel function for the odd eigenfunction and the zeros $\{\tilde{b}_n\}$ of its first derivative for the even solution,

$$J_{b_n}(a)=0 \quad \text{and} \quad J'_{\tilde{b}_n}(a)=0, \tag{11}$$

with $\tilde{b}_0>b_0>\tilde{b}_1>b_1>\ldots$. The eigenstates are

$$\psi_n(x)=\mathcal{N}_nJ_{b_n}(ae^{-\alpha|x|/2}) \tag{12}$$

for the eigenenergies $E_n=-U_0b_n^2/a^2$ and

$$\tilde{\psi}_n(x)=\tilde{\mathcal{N}}_nJ_{\tilde{b}_n}(ae^{-\alpha|x|/2}) \tag{13}$$

for the eigenenergies $\tilde{E}_n=-U_0\tilde{b}_n^2/a^2$, where $\tilde{\mathcal{N}}_n$ is another normalization factor. The subset of solutions $\{b_n\}$ coincides with the eigenenergies of $U_I(x)$ because they satisfy the same boundary conditions, $\psi(0)=0$ and $\psi(x\to+\infty)=0$. The extra subset $\{\tilde{b}_n\}$ results from the extra symmetry of the potential $U_{II}(x)=U_{II}(-x)$. The ground state is given by the first root $\tilde{b}_0$ of the even solutions, that is, $\tilde{E}_0=-U_0\tilde{b}_0^2/a^2$.

In contrast to $U_I(x)$, there is always at least one bound state for the symmetric potential $U_{II}(x)$.[6] The threshold a_c below which there is no bound state for $U_I(x)$ can now be interpreted for the extended potential $U_{II}(x)$. The threshold leads to the appearance of the first excited state of $U_{II}(x)$. The comparison between the spectra of $U_{II}(x)$ and $U_I(x)$ gives an example illustrating how boundary conditions influence the existence of at least one bound state for a one-dimensional potential.

C. Scattering states of $U_{II}(x)$

The scattering states are obtained for $E>0$ ($b=i\beta$ is purely imaginary, $\beta>0$) and are discussed here only for $U_{II}(x)$. An incident plane wave coming from $-\infty$ gives rise to reflected and transmitted waves. The asymptotic expansion for large $|x|$ of Eq. (10b) yields

$$\psi(x)\simeq A_1^+\left(\frac{a}{2}\right)^b\frac{e^{-ikx}}{\Gamma(1+b)}+A_2^+\left(\frac{a}{2}\right)^{-b}\frac{e^{ikx}}{\Gamma(1-b)}, \tag{14a}$$

$$\psi(x)\simeq A_1^-\left(\frac{a}{2}\right)^b\frac{e^{ikx}}{\Gamma(1+b)}+A_2^-\left(\frac{a}{2}\right)^{-b}\frac{e^{-ikx}}{\Gamma(1-b)}, \tag{14b}$$

where the Γ function is defined by $\Gamma(z)=\int_0^\infty t^{z-1}e^{-t}dt$. We infer the reflection probability $|r|^2$ as a function of the dimensionless parameters a and b by setting $A_1^+=0$,

$$|r|^2=\left|\frac{A_2^-}{A_1^-}\right|^2=\frac{1}{4}\left|\frac{J_b(a)}{J_{-b}(a)}+\frac{J'_b(a)}{J'_{-b}(a)}\right|^2. \tag{15}$$

The result, as shown in Fig. 2, exhibits reflection for small values of β due to the fast variation of the de Broglie wavelength $\lambda_{dB}(x)=h/mv(x)$ as β approaches zero,

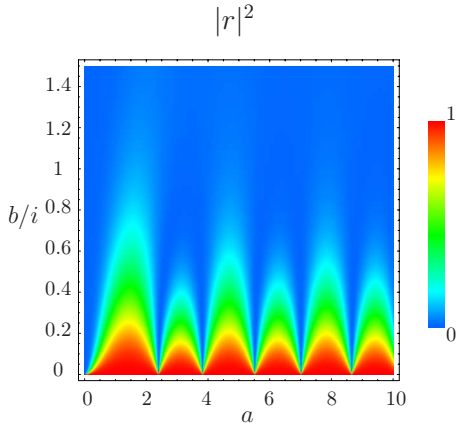

Fig. 2. (Color online) Reflection probability $|r|^2$ for the scattering states of the potential $U_{II}(x)$ as a function of the dimensionless parameters a and b. The large reflection domains at low energy (low $\beta=b/i$) are a signature of quantum reflection. The periodic structure is a matter-wave Fabry–Pérot-like effect.

$$\max\left(\frac{d\lambda_{dB}}{dx}\right)=\frac{4\pi}{3\sqrt{3}}\frac{1}{\beta}\underset{\beta\to 0^+}{\to}+\infty. \tag{16}$$

The reflection probability displays a periodic structure as a function of a, which is caused by a Fabry–Pérot cavity-like resonance effect of the matter wave between the walls of the potential well.

III. THE SUPERSYMMETRY FORMALISM AND ITS APPLICATION TO EXPONENTIAL POTENTIALS

Supersymmetry (SUSY) applied to one-dimensional problems in quantum mechanics allows us to construct a family of exactly solvable Hamiltonians from a given solvable problem.[3] In this section, we give a brief discussion of this method and illustrate it for exponential potentials.

We consider the Hamiltonian $H=T+V(x)$, where $T=-(\hbar^2/2m)d^2/dx^2$ is the kinetic energy term and $V(x)$ is the potential energy term. The eigenvalues and eigenfunctions for the bound states satisfy $H|\psi_n\rangle=E_n|\psi_n\rangle$, with $n=0,1,2,\ldots$. We introduce the potential $V_-(x)=V(x)-E_0$. The corresponding Hamiltonian $H_-=T+V_-(x)$ has the same eigenfunctions, $|\psi_n^-\rangle=|\psi_n\rangle$ as H, and its eigenenergies, $E_n^-=E_n-E_0$, are translated with respect to those of H and are therefore positive ($E_n^-\geq 0$),

$$H_-|\psi_n^-\rangle=E_n^-|\psi_n^-\rangle. \tag{17}$$

The ground state of H_- has zero energy, $H_-|\psi_0^-\rangle=0$, so that

$$V_-(x)=\frac{\hbar^2}{2m}\frac{\psi_0''(x)}{\psi_0(x)}, \tag{18}$$

where $\psi_0''(x)$ is the second derivative of the ground state wave function, $\psi_0(x)$, with respect to the variable x. The Hamiltonian H_- can thus be recast in the form

$$H_-=-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}-\frac{\psi_0''(x)}{\psi_0(x)}\right). \tag{19}$$

In this form the Hamiltonian can be factorized, that is, written as $H_-=A^+A^-$, where we have introduced the operators

$$A^\pm=-\frac{\hbar}{\sqrt{2m}}\left(\pm\frac{d}{dx}+\frac{\psi_0'(x)}{\psi_0(x)}\right). \tag{20}$$

This factorization can be viewed as a generalization of the one developed for the analysis of the one-dimensional harmonic oscillator.[8]

We introduce the superpotential[2]

$$W(x)=-\frac{\hbar}{\sqrt{2m}}\frac{\psi_0'(x)}{\psi_0(x)}. \tag{21}$$

This potential is defined over the domain of values for which $V(x)$ remains finite. It has no divergence on this domain because the ground state wave function $\psi_0(x)$ has no nodes. The relation between the superpotential $W(x)$ and $V_-(x)$ is by definition

$$V_-(x)=W^2(x)-\frac{\hbar}{\sqrt{2m}}W'(x). \tag{22}$$

This relation suggests that we introduce another potential defined as

$$V_+(x)=W^2(x)+\frac{\hbar}{\sqrt{2m}}W'(x). \tag{23}$$

The Hamiltonian $H_+=T+V_+(x)$ can also be simply expressed in terms of the operators $A^\pm$: $H_+=A^-A^+$.

The spectra (17) of H_- and H_+ are closely related. If we use the expression for $H_\pm$ in terms of the operators $A^\pm$, we can readily show that

$$H_-A^+|\psi_n^+\rangle=E_n^+A^+|\psi_n^+\rangle, \tag{24a}$$

$$H_+A^-|\psi_n^-\rangle=E_n^-A^-|\psi_n^-\rangle. \tag{24b}$$

Because $E_0^-=0$, we conclude that $A^-|\psi_n^-\rangle$ for $n\neq 0$ are eigenstates of H_+ for the eigenvalues E_n^-. We can therefore write $|\psi_m^+\rangle=A^-|\psi_n^-\rangle$, so that $E_m^+=E_n^-$. Except for the ground state E_0^-, all the eigenenergies of H_- and H_+ coincide: $E_n^+=E_{n+1}^-$. Starting from a given solvable potential with N_b bound states, we can thus construct by iteration a new set of N_b exactly solvable potentials having, respectively, N_b-1, $N_b-2,\ldots,0$ bound states.

Supersymmetry also permits us to relate the reflection and transmission coefficients when the two partner potentials, $V_\pm$, have continuous spectra. Let us assume for simplicity that the potentials $V_\pm$ are defined over the entire real axis, and that the superpotential obeys the boundary conditions $W(x\to\pm\infty)=0$.[11] It follows that $V_\pm(x\to\pm\infty)=0$. We consider an incident plane wave e^{ikx} of energy $E=\hbar^2k^2/2m$ coming from $x\to-\infty$. The scattering states that account for the reflected and transmitted waves are

$$\psi^\pm(k,x\to-\infty)\sim e^{ikx}+r^\pm(k)e^{-ikx}, \tag{25a}$$

$$\psi^\pm(k,x\to+\infty)\sim t^\pm(k)e^{ikx}. \tag{25b}$$

If we use Eqs. (24) and (25), we find $r_+(k)=-r_-(k)$ and $t_+(k)=t_-(k)$, which implies that the partner potentials have identical reflection and transmission probabilities $[|r_+(k)|^2=|r_-(k)|^2$ and $|t_+(k)|^2=|t_-(k)|^2]$.

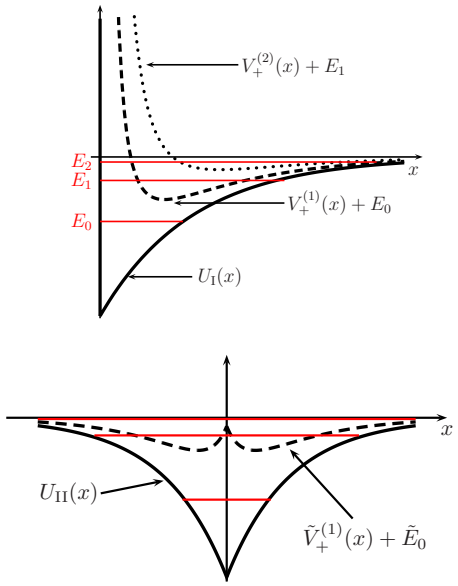

Fig. 3. (Color online) (a) The potential $U_{\rm I}(x)$ with three bound states and its first two supersymmetric partners $V_+^{(1)}(x)+E_0$ and $V_+^{(2)}(x)+E_1(a=11.75)$. (b) $U_{\rm II}(x)$ with three bound states and its first supersymmetric partner $\tilde{V}_+^{(1)}(x)+\tilde{E}_0$, which has a double well shape ($a=4.5$).

A. Application to $U_{\rm I}(x)$

To use the formalism of supersymmetry, we introduce the potential $V_-^{(1)}(x)=U_{\rm I}(x)-E_0$ and deduce from Eq. (21) the corresponding superpotential $W^{(1)}$,

$$W^{(1)}(x)=\sqrt{U_0}e^{-\alpha x/2}\frac{J'_{b_0}(ae^{-\alpha x/2})}{J_{b_0}(ae^{-\alpha x/2})}, \tag{26}$$

and the potential $V_+^{(1)}(x)=2[W^{(1)}(x)]^2+E_0-U_{\rm I}(x)$. $V_+^{(1)}(x)$ is a smooth potential that behaves as $\sim x^{-2}$ as $x\to 0$ and decays as $\exp(-\alpha x)$ for $\alpha x\gg 1$ [see Fig. 3(a)].[12] Similarly, we introduce $V_-^{(2)}(x)=V_+^{(1)}(x)-(E_1-E_0)=2[W^{(1)}(x)]^2-U_{\rm I}(x)+2E_0-E_1$, whose ground state wave function is

$$\psi_0^{(2)}\propto A^-\psi_1\propto\psi'_1-\frac{\psi'_0\psi_1}{\psi_0}, \tag{27}$$

from which we deduce the explicit form of the superpotential,

$$W^{(2)}=-\frac{\hbar}{\sqrt{2m}}\frac{\psi_0(\psi_0\psi''_1-\psi''_0\psi_1-\psi'_0\psi'_1)+\psi'_0\psi'_0\psi_1}{\psi_0(\psi_0\psi'_1-\psi'_0\psi_1)}. \tag{28}$$

As before, the potential $V_+^{(2)}(x)=2[W^{(2)}(x)]^2-V_-^{(2)}(x)$ has the same spectrum as $V_-^{(2)}(x)$ except for the ground state. In Fig. 3(a), we plot $U_{\rm I}(x)$ for $a=11.75$, $\alpha=1$, and show that this potential has three bound states ($N_b=3$). We have also plotted the supersymmetric partners $V_+^{(1)}(x)+E_0$, whose two bound states correspond to the first two excited states of $U_{\rm I}(x)$, and $V_+^{(2)}(x)+E_1$, whose unique bound state corresponds to the second excited state of $U_{\rm I}(x)$.

B. Application to $U_{\rm II}(x)$

The supersymmetric potential associated with $U(x)$ is directly deduced from the ground state wave function $\tilde{\psi}_0(x)$,

$$W^{(1)}(x)=\mathrm{sgn}(x)\sqrt{U_0}e^{-\alpha|x|/2}\frac{J'_{\tilde{b}_0}(ae^{-\alpha|x|/2})}{J_{\tilde{b}_0}(ae^{-\alpha|x|/2})}. \tag{29}$$

Interestingly, we can derive the entire supersymmetric family as in the previous example starting from a potential that has a singularity in its first derivative.[13] From Eq. (21), we observe that if the potential has the differentiability class $\mathcal{C}^n$ (the n first derivatives exist and are continuous), the supersymmetric potential has a differentiability class $\mathcal{C}^{n+1}$. If we repeat the same procedure as before, we readily derive the family of supersymmetric potential partners $\{\tilde{V}_+^{(n)}\}$ of $U(x)$ [see an example in Fig. 3(b)]. The supersymmetric partner $\tilde{V}_+^{(1)}$ has a double well shape. Supersymmetry applied to the potential $U_{\rm II}(x)$ thus generates a family of exactly solvable double well potentials. This connection between single well and double well supersymmetric partners is discussed in Ref. 14. We note that there are not many examples of analytically solvable double well potentials. We mention, for instance, the potentials of the form $V(x)=k(|x|-a)^2$.[15]

The scattering reflection and transmission probabilities for the potential $\tilde{V}_+^{(1)}(x)$ are the same as those for the potential $U_{\rm II}(x)$. In particular, Eq. (15) gives the reflection probability for any value of the parameter a.

IV. APPROXIMATION METHODS

So far, the results we have obtained are exact. In the following, we approximate the ground state energy of $U_{\rm I}(x)$ and $U_{\rm II}(x)$ using the variational method and check the accuracy of this method and test the accuracy of various semiclassical quantization formulas for the whole spectrum.

A. The variational method

To implement the variational method, we choose a set of trial wave functions $\{\varphi_\sigma(x)\}$. We will consider a family of trial wave functions that depend on the parameter σ. The minimum of the expectation value of the Hamiltonian $H=p^2/2m+U(x)$ for these trial functions gives an upper bound for the ground state energy. The functional form of the trial ground state has to be chosen appropriately to obtain a good approximation of the ground state energy E_0,

$$\min_\sigma(\langle\varphi_\sigma|H|\varphi_\sigma\rangle)\geq E_0. \tag{30}$$

1. Application to $U_{\rm I}(x)$

Because $U_{\rm I}(x)$ has an infinite repulsive barrier at $x=0$, the ground state wave function vanishes at $x=0$. We first choose the family of functions,

$$\varphi_\sigma(x)=\left(\frac{2}{\pi}\right)^{1/4}\frac{x}{\sigma^{3/2}}e^{-x^2/4\sigma^2}, \tag{31}$$

which is normalized to unity and obeys the same boundary condition $\varphi_\sigma(0)=0$ and $\varphi_\sigma(+\infty)=0$ as the ground state. This guess is inspired by the first excited wave function of the

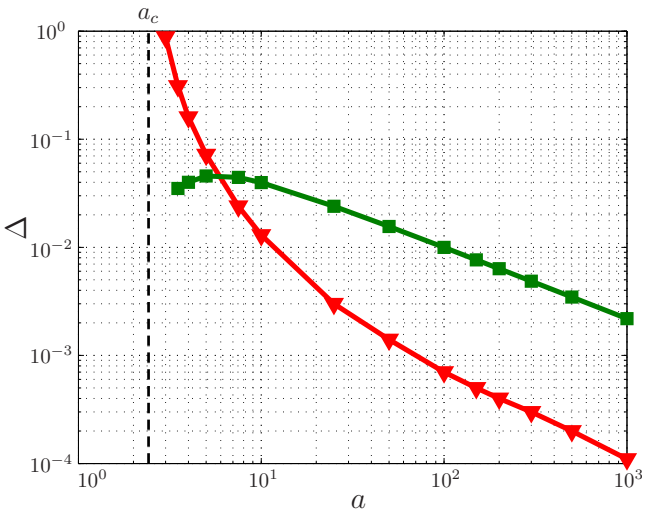

Fig. 4. (Color online) The relative error, $\Delta=|E_{\text{exact}}-E_1(\eta_0)|/|E_{\text{exact}}|$, of the estimate of the ground state energy using the Gaussian ansatz in Eq. (35) $\{\varphi_\sigma\}$ (triangles), and the exponential ansatz $\{\bar{\varphi}_\sigma\}$ (squares) as a function of the dimensionless parameter a. For a less than the critical value $a_c \simeq 2.405$, the $U_{\text{I}}(x)$ does not accommodate any bound states. At the crossing of the square and triangle curves, the well is still shallow and accommodates only two bound states.

one-dimensional harmonic oscillator. We now have to calculate the expectation value of H for the wave functions $\{\varphi_\sigma(x)\}$. This quantity is a function of U_0 and the dimensionless variables a and $\eta=\alpha\sigma/\sqrt{2}$,

$$E_{\text{I}}(\eta)=\langle\varphi_\sigma|H|\varphi_\sigma\rangle=E_c(\eta)+E_p(\eta). \tag{32}$$

We find

$$E_c(\eta)=\frac{\hbar^2}{2m}\int_0^\infty\left|\frac{\mathrm{d}\varphi_\sigma}{\mathrm{d}x}\right|^2\mathrm{d}x=\frac{\hbar^2}{2m}\frac{3}{4\sigma^2}=\frac{3U_0}{2a^2\eta^2}, \tag{33a}$$

$$E_p(\eta)=-U_0\left[e^{\eta^2}(1+2\eta^2)\mathrm{erfc}(\eta)-\frac{2\eta}{\sqrt{\pi}}\right]. \tag{33b}$$

The minimization of the total energy is obtained for $\eta=\eta_0$, which depends only on a,

$$\left.\frac{\mathrm{d}E_{\text{I}}}{\mathrm{d}\eta}\right|_{\eta_0}=0 \quad \text{with} \quad \left.\frac{\mathrm{d}^2E_{\text{I}}}{\mathrm{d}\eta^2}\right|_{\eta_0}>0. \tag{34}$$

Figure 4 compares the relative error $\Delta=|E_{\text{exact}}-E_{\text{I}}(\eta_0)|/|E_{\text{exact}}|$ of the estimate of the ground state energy as a function of a. The poor accuracy for small U_0 is due to the inappropriate functional form of the trial function that does not reproduce well the large extension of the wave function for small a. This interpretation can be confirmed by using the family of normalized wave functions of the form $\bar{\varphi}_\sigma(x)=2xe^{-x/\sigma}/\sigma^{3/2}$. These wave functions have a longer tail for large x than those of $\{\varphi_\sigma(x)\}$ and yield a better estimate for the energy for small low a, that is, for a small trap depth as illustrated in Fig. 4. The variational method allows an approximate determination of the threshold value a_c below which there is no bound states. We find $a_c^{\text{var}}\simeq 2.5142$ as the lowest bound of a above which a solution of the equivalent of Eq. (34) for the family $\{\bar{\varphi}_\sigma(x)\}$ exists. This value differs by $\approx 4.5\%$ from the exact value. If U_0 is increased, the wave function becomes more localized, and the estimate for the ground state energy is much better with the trial wave functions of the family $\{\varphi_\sigma(x)\}$, as shown in Fig. 4.

2. *Application to* $U_{\text{II}}(x)$

The minimization of the Hamiltonian expectation value for the potential $U_{\text{II}}(x)$ is performed in the subspace of Gaussian trial functions,

$$\tilde{\varphi}_\sigma(x)=\left(\frac{1}{2\pi}\right)^{1/4}\frac{1}{\sigma^{1/2}}e^{-x^2/4\sigma^2}. \tag{35}$$

This family of trial functions is inspired by the ground state wave function of the one-dimensional harmonic oscillator and has no node as expected for the ground state of a potential well. We find, for example, $E(\eta_0)\simeq -0.545U_0$ for $a=5$, which differs from the exact value by about 1%.

The variational method also allows for the determination of the first excited state. For this purpose, we have to choose a family that has the same symmetry as the state considered and is orthogonal to the family of states used for the determination of the ground state. The extension of the trial functions used for $U_{\text{I}}(x)$ to the family $\{\hat{\varphi}_\sigma(x\geq 0)=\varphi_\sigma(x)$ and $\hat{\varphi}_\sigma(x\leq 0)=-\varphi_\sigma(-x)\}$ provides a new family that is orthogonal to the family $\{\tilde{\varphi}_\sigma\}$, has one node, and is thus appropriate for the determination of the first excited state by the variational method. This calculation is exactly the one performed on the half space $x\geq 0$ for $U_{\text{I}}(x)$, whose accuracy is summarized for an example in Fig. 4. Thus, the search for an approximation to the ground state energy of $U_{\text{I}}(x)$ using the variational principle gives an estimate of the first excited state of the symmetric extension $U_{\text{II}}(x)$ of $U_{\text{I}}(x)$.

B. Semiclassical quantization formulas

To obtain an approximate determination of the entire spectrum, we rely on semiclassical quantization methods. The most commonly used is the Wentzel–Kramers–Brillouin (WKB) quantization condition.[16–20] We use here the Einstein–Brillouin–Keller quantization approach, which properly takes into account the boundary conditions[19,21,22]

$$\oint p\mathrm{d}x=\left(n+\frac{\nu}{4}\right)h, \tag{36}$$

where ν is the Maslov index that accounts for the total phase loss during one period in units of $\pi/2$.[23,24] A smooth wall gives a contribution to ν of 1 and a sharp wall of 2.[25] For $U_{\text{I}}(x)$, there is a sharp wall at $x=0$ and a smooth one for $x>0$ so that $\nu=1+2=3$. The calculation of the action $\oint p\mathrm{d}x$ for $U_{\text{I}}(x)$ combined with Eq. (36) gives an implicit equation for the eigenenergies,

$$\left(n+\frac{3}{4}\right)\frac{\pi}{a}=F(y_n), \tag{37}$$

with $F(y)=\sqrt{1-y^2}-y\cos^{-1}(y)$, $y_n=\exp(-\alpha x_n/2)$, and $U(x_n)=E$. Semiclassical approaches are supposed to work better for large quantum numbers. We compare in Fig. 5 the exact energies of $U_{\text{I}}(x)$ with $a=32$ and $\alpha=1$ such that $U_{\text{I}}(x)$ accommodates ten bound states with the approximate values obtained from Eq. (37). We observe an accuracy which gets better up to the fifth level but then gets worse.

The standard WKB estimate for the energies is significantly improved by taking into account higher order correc-

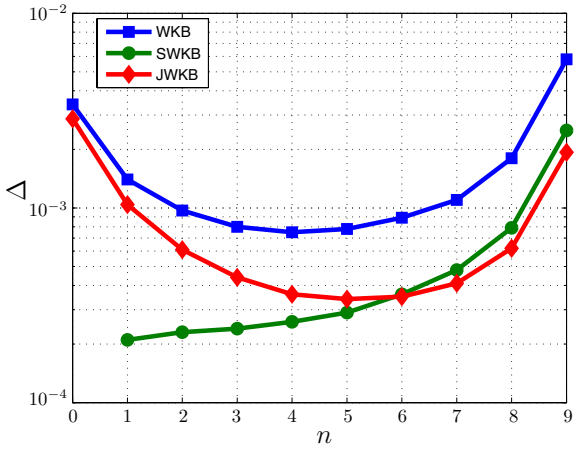

Fig. 5. (Color online) Comparison of WKB (squares), SWKB (disks), and JWKB (diamonds) predictions for the energy spectrum of $U_I(x)$ with $a=32$ (ten bound states) with the exact results. The relative error Δ is plotted for the ten bound states as a function of a.

tions in $\hbar$ to the standard WKB quantization condition. This approximation method is referred to as the JWKB quantization condition.[27] The first correction, δ, is given by

$$\left(n+\frac{\nu}{4}\right)=\frac{1}{h}\oint p\mathrm{d}x+\delta, \tag{38}$$

where

$$\delta=-\frac{1}{24\pi}\left(\frac{\hbar^2}{2m}\right)^{1/2}\frac{\partial}{\partial E}\left(\int_{x_1}^{x_2}\frac{U''(x)}{[E-U(x)]^{1/2}}\mathrm{d}x\right). \tag{39}$$

We use the explicit form of $U_I(x)$ to obtain

$$\left(n+\frac{3}{4}\right)=F(y_n)-\frac{1}{12\pi a\sqrt{1-y_n}}. \tag{40}$$

Compared to the WKB results, we obtain an improved accuracy for the entire spectrum (see Fig. 5).

If we combine the supersymmetry formalism with the WKB method, we can work out the SWKB quantization condition.[28–30] This semiclassical quantization formula reads as

$$\int_{x_{\min}}^{x_{\max}}(2m[E_n^-W^2(x)])^{1/2}\mathrm{d}x=n\hbar\pi, \tag{41}$$

where $x_{\min}$ and $x_{\max}$ are the turning points for the $W^2(x)$ potential defined by $E_n^-=W^2(x_{\min})=W^2(x_{\max})$. The SWKB approach yields the exact bound state spectra for all shape invariant potentials, that is, when the pair of the SUSY partners V_+ and V_- are similar in shape and differ only in the parameters.[31,32] The potential $U_I(x)$ is not shape invariant and, thus, provides an interesting example of the accuracy of the SWKB spectrum prediction. By construction, the SWKB approach requires knowledge of the ground state wave function and, thus, gives the exact ground state energy. As a result, it provides the best estimate for the deep energy states, as shown in Fig. 5. Among the three semiclassical approximation methods we have discussed, the JWKB expression turns out to be the most accurate for the states near the continuum. These conclusions on the relative range of validity and accuracy of the various semiclassical quantization expressions are general.

We consider the highest bound state for a deeper potential.[34] For the WKB, JWKB, and SWKB approximation methods, the deeper the last bound state, the better the estimate. The JWKB method systematically gives a better account of the energy of the last state. This result is well known in molecular physics.[27] The JWKB quantization condition for the highest vibrational levels of a molecular potential can be further improved using the Gribakin and Flambaum formula[33] for the scattering length.[35,36]

The WKB quantization rule for $U_{II}(x)$ yields

$$\left(n+\frac{1}{2}\right)\frac{\pi}{2a}=F(y_n), \tag{42}$$

where $y_n=\exp(-\alpha x_n/2)$ and $U(x_n)$ is the energy of the nth state. Because $U_{II}(x)$ has two smooth walls, $\nu=1+1=2$. As expected, the odd values of n coincide with the energies determined by applying the WKB quantization condition to $U_I(x)$ [see Eq. (37)]. This example provides illustrates the importance of the Maslov index. An extra subset of energies is obtained that corresponds to the even values of n, including the ground state $n=0$, which has an energy lower than the ground state for $U_I(x)$ (see Fig. 1).

V. DISCUSSION

We have discussed the application of supersymmetry to the potentials $U_I(x)$ and $U_{II}(x)$, and illustrated the importance of exact solutions to test approximate methods. The same approach can be used to analyze the family of potential wells of the form $|x|$ defined either on the positive real axis as U_I or on the whole real axis as U_{II}. In addition to the pedagogical value of these examples, a discussion of supersymmetry complements the traditional teaching of quantum mechanics at the undergraduate level. It answers such basic and important questions as can two potential wells have the same spectrum and different shape? Is it possible to construct the potential shape knowing its reflection and transmission probabilities for all incident energies? Does there exist a transparent potential? It generalizes the factorization procedure of the stationary Schrödinger equation introduced for the harmonic oscillator, enlarges the class of exactly solvable potentials, and provides new approximation methods for quantization rules.

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