

Variational method for the double-well anharmonic oscillator

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The independent-minimization variational method is extended to cases with more than one variational parameter and applied to the anharmonic-oscillator problem. The results, including estimates of the tunneling effect, are reasonable. For the double-well potential the method provides a criterion to decide, given the coupling parameter λ , up to which energy level a classical broken-symmetry solution is present. Above that level the symmetry is restored. A lower bound for the value of λ allowing for symmetry-broken solutions is also obtained.

I. INTRODUCTION

Recently, variational methods have been applied to the quantum mechanics of quarkonium systems. In particular, the independent-minimization variational method developed in Refs. 1 and 2 satisfies for each level the virial and Feynman-Hellman theorems, and can thus be used in estimating, with good accuracy, the energy levels and the constituent-mass dependence of energy-level differences.

We have recently learned that many years ago the method was applied to the quantum-mechanical anharmonic oscillator by McWeeney and Coulson.³ In the present work we would like to discuss again the anharmonic oscillator but now with particular emphasis on the double-well anharmonic-oscillator problem.

Our analysis requires the extension of the method by introducing a second variational parameter. In usual calculations one variational parameter K_n , fixed independently for each level and controlling the size of the wave function, has to be introduced. For the problem of finding where to locate the wave function (the case of a potential with several minima and maxima or a potential not symmetric around a minimum) a second variational parameter X_n , controlling the position of the wave function, is required.

In the example of the double-well potential, Fig. 1, simultaneous minimization of the matrix elements $\langle \psi H \psi \rangle_n$ with respect to K_n and X_n provides a criterion to determine, for each level, which kind of solution to choose: either a classical symmetry-broken solution ($\langle x \rangle_n \neq 0$) or a symmetric solution ($\langle X \rangle_n = 0$). Given the value of the coupling parameter λ [in the $(\lambda/4)x^4$ term] we can estimate how many levels correspond to a broken-

symmetry solution and above which level the symmetry is restored. The calculation of energy levels and energy splittings due to tunneling is, in comparison with accurate numerical results, rather acceptable.

We note that the anharmonic-oscillator problem (normal situation or double-well potential) has received great attention in recent years, in particular in connection with the nonconverging character of the coupling-parameter- λ perturbation expansion and the developing of better converging expansions.⁴ On the other hand, path-integral techniques for computing tunneling effects and reproducing WKB results have also been of theoretical interest.⁵ The variational calculations developed here, being of nonperturbative nature, give reasonable answers both in weak- and strong-coupling- λ limits, describe well the broken-symmetry spec-

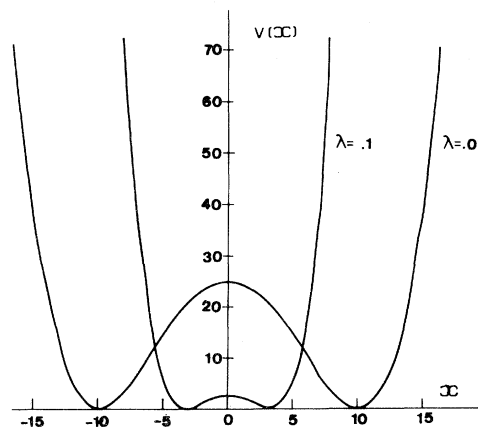


FIG. 1. The double-well anharmonic oscillator and its variation with the coupling parameter λ : $V(x) = (\lambda/4)(x^2 - 1/\lambda)^2$.

trum, and even tunneling is fairly well reproduced.

The rest of the paper is organized as follows. In Sec. II we introduce the two-parameter independent-minimization variational method. In Sec. III we discuss applications, the anharmonic oscillator, and the double-well anharmonic oscillator. In Sec. IV we briefly present our conclusions.

II. VARIATIONAL METHOD WITH TWO PARAMETERS

The idea in the variational method is to estimate the eigenvalues of the nonrelativistic Hamiltonian

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

using the eigenfunctions $\psi(x)$ corresponding to a soluble Hamiltonian H_0 ,

$$H_0 = -\frac{1}{2m} \frac{d^2}{dx^2} + V_0(x). \tag{2}$$

Such estimates are done independently for each eigenstate. In practice, one introduces energy-level-independent variational parameters K_n^i , to be fixed by minimization conditions,

$$\frac{\partial}{\partial K_n^i} \langle \psi H \psi \rangle_n = 0, \quad n = 0, 1, 2, \dots, \quad i = 1, 2, \dots \tag{3}$$

In simple problems only one variational parameter, controlling the size of the wave function, is in-

TABLE I. Examples of radial reduced wave functions written in the form of Eq. (4). The quantities N_n are appropriate normalization factors: $\int u^2(r) dr = 1$. The functions L_n , Ai, and H_{2n+1} are the Legendre polynomials, the Airy function, and Hermite polynomials, respectively. The quantities ϵ_n are the zeros of the Airy function.

Potential	Reduced radial wave functions	Variational parameter K
Coulomb $V = -\frac{e}{r}$	$N_n \sqrt{K} \xi L_n^1(2\xi/n)$	me^2
Linear $V = \lambda r$	$N_n \sqrt{K} \text{Ai}(\xi - \epsilon_n)$	$(2m\lambda)^{1/3}$
Harmonic oscillator $V = \frac{1}{2} m \omega^2 r^2$	$N_n \sqrt{K} e^{-\xi^2/2} H_{2n+1}(\xi)$	$(m\omega)^{1/2}$

roduced. Using the scaling properties of the Schrödinger equation, if V_0 is power behaved and is renormalized and rescaled it is easily shown that the eigenfunctions have the form²

$$\psi_n(x) = \sqrt{K_n} \bar{\psi}_n(\xi) \quad (\xi \equiv K_n x) \tag{4}$$

with normalization

$$\int_{-\infty}^{\infty} \psi_n^2(x) dx = \int_{-\infty}^{\infty} \bar{\psi}_n^2(\xi) d\xi = 1. \tag{5}$$

Most of the soluble examples of the Schrödinger equation—for instance, Coulomb, linear, harmonic-oscillator potentials—correspond to power-behaved potentials. Examples of scaling eigenfunctions are given in Table I. The quantity K_n , conjugate to x , $K_n^{-1} \sim (\langle x^2 \rangle_n)^{1/2}$, is the natural quantity to choose as a variational parameter. For this parameter the minimization condition (3) gives, using (4),

$$\frac{\partial}{\partial K_n} \langle \psi H \psi \rangle_n = \frac{1}{K} \left[2 \langle T \rangle_n - \left\langle x \frac{\partial V}{\partial x} \right\rangle_n \right] = 0, \tag{6}$$

$$2 \langle T \rangle_n = \left\langle x \frac{\partial V}{\partial x} x \right\rangle_n. \tag{7}$$

In other words, the minimization condition (6) is equivalent to imposing the virial theorem. This is the best argument in favor of the method. As the virial theorem is an exact operator relation, true for each level, the independent minimization is in this way justified. On the other hand, as the levels are independently determined, the K_n values differ from level to level and the orthogonality of the wave functions is violated. One should then be cautious when using the method for computation of transition matrix elements.

We consider next, in one space dimension, the situation when the trial potential $V_0(x)$ is, for instance, symmetric under reflection, $V_0(x) = V_0(-x)$, while the potential under study $V(x)$ is not symmetric, $V(x) \neq V(-x)$. This occurs when the potential $V(x)$ is intrinsically not symmetric [for instance, $V(x) = ax + bx^2$], or when it is displaced away from the origin. In such situations trial wave functions centered at the origin, $x = 0$, are not appropriate. One then needs to introduce a second parameter X_n , related to the position of the wave function, and the trial wave functions are then written, generalizing (4), in the form

$$\psi_n(x) = \sqrt{K_n} \bar{\psi}_n[\xi \equiv K_n(x - X_n)]. \tag{8}$$

We note that it is possible to give a perhaps

more transparent physical meaning to X_n and K_n by looking at the first moments of the probability distributions $\psi_n^2(x)$:

$$\langle X \rangle \equiv X_n,$$

$$D_n^2 \equiv \langle x^2 \rangle_n - \langle x \rangle_n^2 \sim 1/K_n^2.$$

The minimization conditions now read

$$\frac{\partial \langle \psi H \psi \rangle_n}{\partial K_n} = \frac{1}{K} \left[2 \langle T \rangle_n - \left\langle x \frac{\partial V}{\partial x} \right\rangle \right] + \frac{1}{K_n} X_n \frac{\partial}{\partial X_n} \langle V(x) \rangle_n = 0, \quad (9)$$

$$\frac{\partial \langle \psi H \psi \rangle_n}{\partial K_n} = \frac{\partial}{\partial X_n} \langle V(x) \rangle_n = 0. \quad (10)$$

One notices that (9) and (10) still ensure that the virial theorem is satisfied. If the potential $V(x)$ is symmetric around a minimum at $x=a$, the solution of (10) is clearly $X_n=a$, with X_n independent of n . If the potential is not symmetric around a minimum at $x=a$, then X_n varies from level to level.

In the cases when the potential has several minima and maxima the second stability condition (10) has to be better analyzed. In particular the acceptable values of X_n are the ones that satisfy (10) and

$$\frac{\partial^2}{\partial X_n^2} \langle V \rangle_n > 0. \quad (11)$$

For the double-well potential Eqs. (10) and (11) select for each level either the broken-symmetry (before tunneling) solution, $X_n \neq 0$, or the symmetry-restored solution, $X_n = 0$.

III. APPLICATIONS

We apply our discussion to the anharmonic-oscillator potential,

$$V(x) = \frac{1}{2} k x^2 + \frac{1}{4} \lambda x^4. \quad (12)$$

The parameter λ is assumed positive, and the parameter k may be either positive (normal anharmonic oscillator) or negative (double-well potential).

For the matrix elements $\langle \psi H \psi \rangle_n$ we have

$$\langle \psi H \psi \rangle_n = -\frac{1}{2m} \left\langle \frac{d^2}{dx^2} \right\rangle_n + \frac{1}{2} k \langle x^2 \rangle_n + \frac{1}{4} \lambda \langle x^4 \rangle_n \quad (13)$$

and, with wave functions (8),

$$\langle \psi H \psi \rangle_n = \frac{1}{2m} A_n K_n^2 + \frac{1}{2} k \left[\frac{B_n}{K_n^2} + X_n^2 \right] + \frac{1}{4} \lambda \left[\frac{C_n}{K_n^4} + \frac{6B_n}{K_n^2} X_n^2 + X_n^4 \right], \quad (14)$$

where the numerical, positive quantities A_n , B_n and C_n are given by

$$A_n \equiv \left\langle -\frac{d^2}{d\xi^2} \right\rangle = \int \bar{\psi}(\xi) \frac{d^2}{d\xi^2} \bar{\psi}(\xi) d\xi, \quad (15)$$

$$B_n \equiv \langle \xi^2 \rangle = \int \xi^2 \bar{\psi}^2(\xi) d\xi, \quad (16)$$

$$C_n \equiv \langle \xi^4 \rangle = \int \xi^4 \bar{\psi}^2(\xi) d\xi. \quad (17)$$

The minimization conditions (9) and (10) read

$$\frac{1}{2m} A_n - \frac{1}{2} k \frac{B_n}{K_n^4} - \frac{1}{2} \lambda \frac{C_n}{K_n^6} - \frac{3}{2} \lambda \frac{B_n}{K_n^4} X_n^2 = 0, \quad (18)$$

$$X_n \left[k + \lambda \left[3 \frac{B_n}{K_n^2} + X_n^2 \right] \right] = 0. \quad (19)$$

With X_n and K_n obtained in this way, substituted back in (13), one estimates the energy E_n of the n th level.

Let us look now at the second condition, Eq. (19). There are two solutions:

$$X_n = 0 \quad (20)$$

and

$$X_n = \pm \left[-\left[\frac{k}{\lambda} + \frac{3B_n}{K_n^2} \right] \right]^{1/2}. \quad (21)$$

If k is positive, normal anharmonic oscillator, the only real solution is, as expected, $X_n = 0$. If k is negative, double-well potential, both solutions can occur. One easily sees that the condition $(\partial^2/\partial X_n^2) \langle \psi H \psi \rangle > 0$ is satisfied if $k/\lambda + 3B_n/K_n^2 > 0$, for the $X_n = 0$ solution, and if $k/\lambda + 3B_n/K_n^2 < 0$, for the $X_n = \pm [-(k/\lambda + 3B_n/K_n^2)]^{1/2}$ solution.

In view of the applications we shall be more specific now. As trial wave functions we use harmonic-oscillator wave functions,

$$\psi_n(x) = N_n \sqrt{K_n} \exp\left[-\frac{1}{2} K_n^2 (x - X_n)^2\right] \quad (22)$$

with

$$N_n = \frac{1}{\pi^{1/4}} \frac{1}{(2^n n!)^{1/2}} \tag{23}$$

The quantities A_n , B_n , and C_n are then

$$A_n = B_n = n + \frac{1}{2} \tag{24}$$

and

$$C_n = \frac{3}{2}(n^2 + n + \frac{1}{2}) \tag{25}$$

A. Normal anharmonic oscillator

The comparison of our estimates with rigorous numerical calculations shows very close agreement. Two examples, one corresponding to weak coupling and the other to strong coupling, are shown in Table II.

For small values of λ our variational method, expanding K_n around the harmonic-oscillator limit, $K_n = 1 + \epsilon\lambda + \delta\lambda^2 + \dots$, and fixing ϵ, δ, \dots by saturation of the minimization condition order by order, gives (putting $m = k = 1$)

$$E_n = (n + \frac{1}{2}) + \frac{3}{2}(n^2 + n + \frac{1}{2})\frac{\lambda}{4} - 2\frac{(n^2 + n + \frac{1}{2})^2}{n + \frac{1}{2}} \left[\frac{\lambda}{4} \right]^2 + \dots \tag{26}$$

An alternating-sign series is, as expected, generated. For the ground state, to first order in λ , we agree with the usual small- λ expansion, but beyond first order we differ (the oscillations are less violent than in the unreliable conventional perturbation expansion).

In the strong-coupling limit the result remains acceptable. For $\lambda \rightarrow \infty$ we obtain ($k = 1, m = 1$)

$$E_n = c_n \lambda^{1/3} = \frac{3}{4} A_n^{2/3} C_n^{1/3} \lambda^{1/3} = \frac{1}{2} (\frac{3}{2})^{4/3} (n + \frac{1}{2})^{2/3} (n^2 + n + \frac{1}{2})^{1/3} \lambda^{1/3} \tag{27}$$

Comparison of the values of c_n for $n = 0, 1, 2$ with detailed calculations is shown in Table III. The differences are less than 2%.

The method thus seems to be reliable in the whole range of λ (weak- and strong-coupling limits) for estimating energy levels.

B. Double-well potential

In order to discuss the double-well potential, Fig. 1, we rewrite (18), after substitution of (21), in the form

$$z^3 - 2mk'z + m\lambda \left[9A_n - \frac{C_n}{A_n} \right] = 0, \tag{28}$$

where $z = K_n^2$ and $k' \equiv -k > 0$. Equation (28) is a third-degree equation whose discriminant is given by

$$\Delta = -(\frac{2}{3}mk')^3 + \left[\frac{m\lambda}{2} \right]^2 \left[9A_n - \frac{C_n}{A} \right]^2 \tag{29}$$

If $\Delta > 0$ there is no acceptable solution (real and positive). If $\Delta < 0$ there is only one real positive

TABLE II. Comparison of the variational method with exact numerical calculations for the anharmonic oscillator, $V(x) = \frac{1}{2}KX^2 + \frac{1}{4}\lambda X^4$, with $K > 0$. Numerical calculations are from Ref. 8.

Quantum number n	$\lambda/(k^3 m)^{1/2} = 0.5$		$\lambda/(k^3 m)^{1/2} \rightarrow \infty$	
	Variational method	Exact calculation	Variational method	Exact calculation
0	0.5120	0.5107	0.6814	0.6680
1	1.6320	1.6263	2.4237	2.3936
2	2.9067	2.9073	4.6850	4.6968
3	4.3006	4.3083	7.2911	7.3367
4	5.7935	5.8098	10.167	10.244
5	7.3722	7.3983	13.267	13.379
6	9.0273	9.0642	16.565	16.712
7	10.752	10.800	20.037	20.221
8	12.540	12.601	23.668	23.890
9	14.387	14.461	27.446	27.706

TABLE III. Asymptotic behavior of the energy levels of the anharmonic oscillator in the $\lambda \rightarrow \infty$ limit. Exact numerical results are from Ref. 9.

n	Asymptotic behavior
	Ratios $\frac{(c_n) \text{ variational method}}{(c_n) \text{ exact calculation}}$
0	1.0201
1	1.0126
2	0.9975

acceptable solution. We thus have the constraint

$$\frac{mk'^3}{\lambda^2} \geq \frac{1}{4} \left(\frac{3}{2}\right)^3 \left[9A_n - \frac{C_n}{A_n}\right]^2 \geq \left(\frac{3}{2}\right)^5 \left[\frac{5n^2 + 5n + 1}{2n + 1}\right]^2. \quad (30)$$

This relation fixes the number of states which correspond classically to a broken-symmetry solution. In particular no such kind of solution exists if

$$\left[\frac{mk'^3}{\lambda^2}\right] \left(\frac{2}{3}\right)^5 < 1. \quad (31)$$

Equation (30) determines, given λ , the number of states corresponding to the broken-symmetry solution, and the value of n above which the symmetry is restored. A plot of λ vs the quantum number n , showing the regions where the symmetric and the

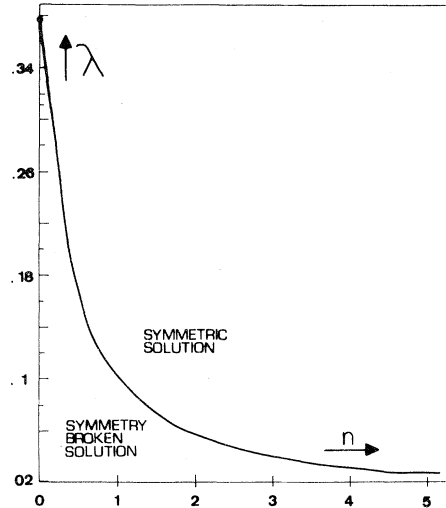


FIG. 2. Phase diagram of λ versus n . Above the line, one has symmetric solutions ($\langle x \rangle_n = 0$), below one has symmetry-broken solutions ($\langle x \rangle_n \neq 0$).

broken-symmetry solutions, respectively, exist, is presented in Fig. 2.

In Table IV we show a comparison of our estimates of the energy levels in the double-well potential with accurate numerical calculations. The zero of the potential is always fixed at the minimum, $V(x) = (\lambda/4)(x^2 - 1/\lambda)^2$. The energy levels lie, as they should, below the harmonic-oscillator values $\sqrt{2}(n + \frac{1}{2})$.

The solutions we have constructed for the double-well potential are not eigenstates of parity. One should then make symmetric and antisym-

TABLE IV. Mean energy levels in the symmetry-broken solution of the double-well oscillator. For values of λ above the ones shown the symmetry is restored. Exact numerical results are from Ref. 7.

λ	Energy levels, E_n (broken-symmetry solution)			
	$n = 0$		$n = 1$	
	Variational	Exact	Variational	Exact
0.02	0.7032	0.7020	2.0783	2.0851
0.04	0.6994	0.6968	2.0311	2.0460
0.06	0.6955	0.6913	1.9781	2.0032
0.08	0.6914	0.6856	1.9158	1.9549
0.1	0.6873	0.6795		
0.14	0.6785	0.6665		
0.20	0.6644	0.6450		
0.30	0.6365	0.6208		
0.34	0.6224	0.6178		

metric combinations of solutions at $X_n = +(k'/\lambda - 3B_n/k_n^2)^{1/2}$ and $X_n = -(k'/\lambda - 3B_n/k_n^2)^{1/2}$, respectively:

$$\begin{aligned}\psi_S &= \alpha_+ [\psi(x) + \psi(-x)], \\ \psi_A &= \alpha_- [\psi(x) - \psi(-x)],\end{aligned}\quad (32)$$

where α_+ and α_- are normalization constants, with $\alpha_+^2 = \alpha_-^2 = \frac{1}{2}$ in the $\lambda \rightarrow 0$ limit.

In order to estimate the energy splitting due to tunneling we can use the approximate known formula,⁶

$$\Delta E = E_A - E_S \simeq \frac{2}{m} \psi(0) \psi'(0). \quad (33)$$

However, it is not *a priori* guaranteed that this formula can be safely used in our case because one needs the wave function at $x=0$, far away from the center of the well, and the method is presumably not accurate enough. For the ground state, Eq. (33) becomes, in our scheme,

$$\Delta E_0 = \frac{2k_0^2}{\pi^{1/2}} (K_0 X_0) e^{-(K_0 X_0)^2}. \quad (34)$$

Our results, using Eq. (34) with K_0 and X_0 given by (18) and (21), in comparison with the accurate numerical determinations of Ref. 7, are shown in Fig. 3. The result is quite acceptable, in particular having in mind the several orders of magnitude involved. Qualitatively, our result is similar to the WKB calculation, but while in the WKB scheme one obtained, as $\lambda \rightarrow 0$ ($m=1$),

$$\Delta E_0 \xrightarrow[\lambda \rightarrow 0]{\text{WKB}} 2^{11/4} \left[\frac{k'}{\pi} \right]^{1/2} \left[\frac{k'^{3/2}}{\lambda} \right]^{1/2} \exp \left[-\frac{2\sqrt{2}}{3} \frac{k'^{3/2}}{\lambda} \right], \quad (35)$$

here we have, with $K_0 \sim (2k')^{1/2}$ and $X_0^2 \sim k'/\lambda$,

$$\Delta E_0 \sim 2^{7/4} \left[\frac{k'}{\pi} \right]^{1/2} \left[\frac{k'^{3/2}}{\lambda} \right]^{1/2} \exp \left[-\sqrt{2} \frac{k'^{3/2}}{\lambda} \right] \quad (36)$$

$$\Delta E_0 = E_A - E_S = \left[-\frac{K_0^2}{m} (K_0 X_0)^2 + \frac{k'}{K_0^2} (K_0 X_0)^2 - \frac{\lambda}{4} \left[\frac{3B_0}{K_0^4} (K_0 X_0)^2 + \frac{1}{2k_0^4} (K_0 X_0)^4 \right] \right] e^{-(K_0 X_0)^2}. \quad (38)$$

The results, using this formula, for the energies used in Fig. 2, are similar to the ones plotted and corresponding to Eq. (34).

Finally we note that we could have rigorously—

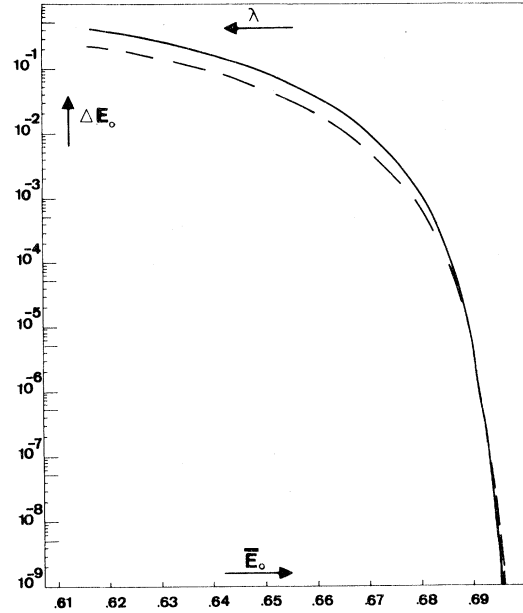


FIG. 3. Tunneling effect. Energy splittings ΔE_0 as a function of mean ground-state energy E_0 . The full line is the variational method prediction with Eq. (33) or (34). The dashed line is the exact numerical calculation of Ref. 8.

and a much faster vanishing of ΔE_0 with λ as $\lambda \rightarrow 0$.

We have tried an alternative estimate of ΔE_0 , by computing directly E_A and E_S , keeping K_n and X_n fixed, using Eqs. (32) and our previous determination of E . For the ground state we have obtained, for α_{\pm} given by

$$\alpha_{\pm}^2 = \frac{1}{2(1 \pm e^{-(K_0 X_0)^2})} \simeq \frac{1}{2} \left[1 \mp e^{-(K_0 X_0)^2} \right], \quad (37)$$

symmetric splittings around E_0 with

within the method—computed ΔE by evaluating E_A and E_S and minimizing with respect to $K_0^{4,S}$ and $X_0^{4,S}$. The formulas however would have not been as simple as (34) or (38).

IV. CONCLUSIONS

We have presented the independent-minimization variational method and argued that, as far as energy levels are concerned, the method is rather accurate. This happens because at each level we force the trial potential to agree, in magnitude and slope in x , with the potential being studied, as a consequence of the virial theorem.

The anharmonic oscillator was discussed as an interesting two-variational parameter example.

The overall result is satisfactory. In the double-well case, $k = k' < 0$, we were able to determine consistently the values of the mean energy of the levels (before tunneling)—and the deviations from the naive harmonic-oscillator limit at the bottom of the well—as well as the energy splittings due to tunneling. Some of our results may be of theoretical interest as, for instance, our bound, Eqs. (30) and (31) and Fig. 2, for the number of levels corresponding classically to a broken-symmetry solution.

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