

Accurate energy levels and partition function of a quantum-mechanical anharmonic oscillator

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An optimized variational method to calculate the energy eigenvalues for the anharmonic oscillator is proposed. The convergence for the single-well potential is very quick; for the double well it decreases as the wells become deeper, and larger matrices should be diagonalized to obtain required accuracy. The partition function and free energy are calculated for the single- and double-well potentials.

The one-dimensional anharmonic oscillator (AO), which can be regarded as a field theory in one dimension,¹ recently became the testing ground for new methods in quantum field theory (QFT), particularly in the case when the solutions of the classical field equations are degenerate. It led to renewed interest in calculating the accurate eigenvalues of the Schrödinger equation

$$H\psi_n(x) = E_n\psi_n(x) \quad (1)$$

with the AO Hamiltonian given by

$$H = \frac{1}{2} \left[\frac{d^2}{dx^2} + \omega^2 x^2 \right] + \lambda x^4. \quad (2)$$

It is convenient to eliminate one parameter, expressing all quantities in the units of an appropriate power of λ . After rescaling $x \rightarrow x\lambda^{-1/6}$, $H \rightarrow H\lambda^{1/3}$, and $\omega \rightarrow \omega\lambda^{1/3}$, the AO spectrum depends on only one dimensionless parameter $z = \frac{1}{2}\omega^2\lambda^{-2/3}$, which accounts for the relative strength of the harmonicity and anharmonicity. When discussing numerical results, we will use the rescaled quantities.

The spectrum of the AO can be studied perturbatively, expanding the AO eigenfunctions and eigenvalues into a series in ϵ for the Hamiltonian which has been divided into the following manner:

$$H = H_0 + \epsilon H_I, \quad (3)$$

where H_0 is an exactly solvable operator. The conventional perturbation series is generated, if the Hamiltonian of the harmonic oscillator (HO) with frequency ω is taken as the unperturbed part

$$H_0 = \frac{1}{2} \left[\frac{d^2}{dx^2} + \omega^2 x^2 \right],$$

and the anharmonicity as a perturbation $H_I = \lambda x^4$. The conventional perturbation series for the AO energies diverges¹ and the Borel sum can be found² only if $\omega^2 > 0$; i.e., the classical potential is single-well (SW) shaped. For the double-well (DW) potential ($\omega^2 < 0$), the series is not even Borel summable.³ Therefore, a different choice of H_0 has been considered, to generate a series with better convergence properties. For a review see Ref. 4.

A linear variational method can be constructed for

every choice of the unperturbed Hamiltonian H_0 , taking its eigenfunctions $\phi_n(x)$ as an orthonormal basis to decompose the AO eigenfunctions:

$$\psi(x) = \sum_{n=1}^{\infty} c_n \phi_n(x). \quad (4)$$

Varying the coefficients c_n , to obtain the minimal expectation value of the Hamiltonian in the normalized state ψ , gives an infinite set of equations:

$$\sum_{m=1}^{\infty} (H_{nm} - E\delta_{nm})c_m = 0. \quad (5)$$

Exact energy levels are obtained after diagonalization of the infinite Rayleigh-Ritz (RR) matrix. Numerical calculations for the truncated set of N basic functions provide approximate values of the N lowest eigenstates. For $N=1$ we can only find the ground-state energy; it coincides with the first-order perturbative result for the partitioning given in Eq. (3). Increasing N , more energy levels are obtained with increasing accuracy and the convergence of the method can be estimated. Such systematic application of the variational method provides an alternative to the perturbative calculations. Generally, the accuracy of the n th eigenvalue decreases, as n approaches the truncation level N . A convergence rate of the variational scheme depends strongly on the choice of basis functions, i.e., on the particular partitioning given in Eq. (3). For the conventional choice of H_0 the convergence decreases with decreasing ω^2 and the method will not be applicable for $\omega^2 < 0$, when the HO spectrum is continuous.

In this work we build the variational scheme on the partitioning

$$H = \frac{1}{2} \left[\frac{d^2}{dx^2} + \Omega^2 x^2 \right] + \epsilon [\lambda x^4 + \frac{1}{2}(\omega^2 - \Omega^2)x^2], \quad (6)$$

used in the Caswell⁵ and Killingbeck⁶ (CK) perturbative method. An arbitrary HO frequency Ω in the unperturbed part has been introduced in such a way that the Hamiltonian becomes equal to the Hamiltonian given in Eq. (2) when $\epsilon=1$. The exact value of any physical quantity, obtained after a series summation, does not depend explicitly on Ω . However, if the series is truncated to the order (k), the dependence on Ω appears. The frequency

Ω can be fixed by the principle of minimal sensitivity (PMS), requiring the dependence on the unphysical parameter Ω be as weak as possible.⁷ In the k th-order CK calculations the parameter Ω is fixed for each energy level (n) independently, requiring

$$\frac{dE_k^n}{d\Omega} = 0. \quad (7)$$

The corresponding set of eigenfunctions is not orthogonal in any finite order. For the SW classical potential, the first-order CK method gives the bound-state energies with the error less than 2%, in the whole range of λ (Refs. 5 and 6). The agreement becomes better in higher orders,⁵ as opposed to the conventional perturbation results, which become worse even for small values of λ , as the series is asymptotic. For the DW potential the CK series seems to be still summable; however, the number of orders necessary to obtain the convergence increases as $z \rightarrow \infty$ (for $z = -3.7$ twenty orders have to be included,⁵ to obtain 2-figure accuracy).

In the variational scheme we use a basis of the HO wave functions

$$|n\rangle = \phi_n(x) = \left[\frac{\Omega}{\sqrt{\pi} 2^n n!} \right]^{1/2} H_n(\Omega x) e^{-\Omega^2 x^2/2}, \quad (8)$$

where $H_n(\Omega x)$ are Hermite polynomials and the scale parameter Ω is arbitrary. Such a variational method has been used first for the quartic oscillator ($\omega=0$) by McWeeny and Coulson,⁸ who stressed the dependence of the convergence rate on the choice of Ω . In the calculations of the n th eigenvalue they proposed to take Ω which minimizes the expectation value of the Hamiltonian in the HO state $|n\rangle$. For the SW oscillator quick convergence for the whole spectrum is obtained by choosing the parameter Ω in the HO basis to minimize the expectation value of the Hamiltonian for the lowest HO eigenstate. For the DW such a method does not work if z is too negative, as has been observed by Balsa, Plo, Esteve, and Pacheco.⁹ They proposed to minimize the value of the Hamiltonian in the n th HO state, treating n and Ω as variational parameters. The RR method with Ω fixed in this way converges quickly, but the scheme lacks a physical interpretation, as the solution corresponds to $n = -\frac{1}{2}$. It was pointed out by Quick and Miller,¹⁰ who proposed instead to minimize the sum of K expectation values, requiring that Ω satisfy

$$\frac{d}{d\Omega} \left[\sum_{n=0}^{K-1} \langle n | H | n \rangle \right] = 0 \quad (9)$$

and treating K as an additional parameter.

However, this method also has no physical interpretation. In the RR method the only variational parameters are the coefficients of the wave-function decomposition in the orthonormal basis. If the basic functions are chosen to have a parametric dependence, their values can be chosen to improve a convergence. To this end all the discussed methods have used the requirement that the expectation values of the AO Hamiltonian in the HO states (or its sum) should be minimal. However, according to the Ritz principle, the quantity which should be minimal is

the expectation value of the Hamiltonian in the AO eigenstate, which is an eigenvalue of the RR matrix, but not its diagonal element nor an arbitrary sum of such elements. To find the AO expectation value, the RR matrix should be diagonalized analytically. If the convergence is quick, one can attempt to find an analytical solution. Similar ideas have been applied to the SW potential providing analytical approximations for the energy eigenvalues that are better than perturbative results.¹¹ However, it is not applicable for large truncation orders, which are necessary to obtain a good convergence in the DW case. For numerical calculations it is more convenient to fix Ω before the diagonalization of the RR matrix. In this case it is better to use the PMS rather than the Ritz principle. The PMS can be applied to any physical quantity, and there is such a quantity which can be calculated before diagonalization of the N th-order RR matrix—it is a trace of this matrix. Because the trace is invariant under diagonalization, it equals the sum of elements of diagonalized matrix, i.e., the sum of N lowest AO eigenvalues in this approximation (neither the sum of $K < N$ nor $K > N$ has this property). As an approximant of the physical quantity the trace should be insensitive to the variation of the unphysical parameter Ω . It gives the requirement (9) with K equal to the truncation order N . Quick and Miller have established numerically that the number of included states K has to be roughly equal to the order N of the variational matrix, to obtain a good convergence. In our approach $K = N$ is an immediate consequence of the application of the PMS to the only physical quantity, which can be found before diagonalization of the RR matrix. As the PMS requirement coincides with the necessary condition for minimum, the numerical results in our approach (applied independently in the sector of even and odd HO functions) are the same as given in Tables I–IV of Ref. 10 in the columns corresponding to $K = N$. The convergence properties are much better than obtained by Balsa, Plo, Esteve, and Pacheco⁹ (diagonalization of the matrix of the order two times smaller gives the same accuracy). For the DW potential as $z \rightarrow -\infty$ the convergence decreases. In this case larger matrices should be considered and the numerical errors limit the accuracy.

As expected in the variational method, the coefficients of the expansion of the eigenfunctions in the HO basis are obtained with a poor accuracy (2–3 figures). However, the accuracy of the measurable matrix elements of the operators x and x^2 is much better. To calculate these elements it is more convenient to treat both parity sectors simultaneously, keeping the basis orthogonal. Application of the PMS to the sum of N even and N odd functions gives the equation for Ω :

$$2N(\Omega^3 - \omega^2\Omega) - 2\lambda(8N^2 + 1) = 0. \quad (10)$$

Taking $2N = 110$ for the quartic oscillator ($\omega=0$) the energies of 70 states converge up to 12 significant figures, and the matrix elements $\langle m | x | n \rangle$ and $\langle m | x^2 | n \rangle$ between 10 lowest states converge up to 8 figures. The results agree within the quoted accuracy with the very accurate results obtained from the recurrence relations resulting from the Hill determinant.¹² A reasonable accuracy can be obtained with the matrix of the order $2N < 130$

even for DW if $|z| < 100$.

The variational method is very convenient to calculate a partition function

$$Z(T) = \sum_{n=0}^{\infty} \exp(-E_n/T), \quad (11)$$

at finite temperature T , as it gives the whole set of energy levels at once. As before, we rescale in terms of the coupling constant λ , i.e.,

$$T \rightarrow T\lambda^{-2/3}.$$

For the SW potential the partition function has been calculated by direct summation of (11), using the eigenvalues obtained variationally,¹³ or approximated analytically.¹⁴ The low- and high-temperature limits have been discussed for derivative thermodynamic quantities. We have calculated the partition function of the AO for the SW as well as the DW potential using the optimized variational method. The required accuracy can be obtained, checking the convergence for the calculated quantity with increasing order of the RR matrix. In Fig. 1 we present the free energy $F = -T \ln Z$ as a function of a temperature for different values of z . Although the shape of the classical potential is qualitatively different for $z > 0$ (SW) and $z < 0$ (DW), the partition function and other thermodynamic quantities depend on the temperature in a very similar way. It can be attributed to the fact that there is no phase transition in quantum mechanics (QM) as the symmetry cannot be spontaneously broken.

The optimized variational method to calculate the spectrum of the Hermitian operator is shown here for the AO. We have used the CK partitioning (6), but every other choice of the unperturbed Hamiltonian, used to generate perturbation series,⁴ can be also applied to generate a variational scheme. Both methods can be optimized with the use of PMS, if H_0 contains arbitrary parameters. Another QM problem can be solved in the same manner.

A similar approach can be applied in QFT, if a functional Schrödinger formulation is used. For scalar theory with $\lambda\phi^4$ interaction it will be a generalization of the QM anharmonic oscillator Schrödinger equation. Using a trial wave functional expressed as a linear combination of the

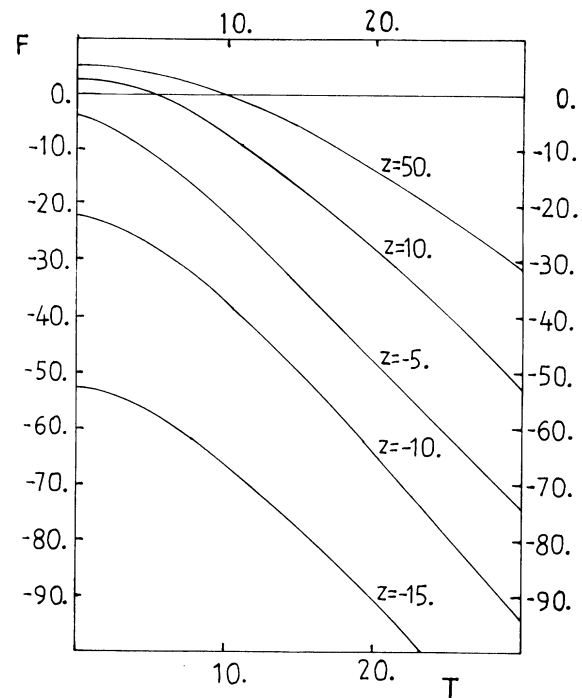


FIG. 1. The free energy F of the anharmonic oscillator, as a function of the temperature T for different values of the parameter $z = \frac{1}{2}\omega^2\lambda^{-2/3}$.

vacuum and multiparticle wave functionals of a free theory with an arbitrary mass Ω , the Ritz principle will determine the best vacuum and multiparticle states functionals and energies of the interacting theory. The quality of the approximation could be improved systematically by increasing the number of multiparticle states of the free theory taken into account.

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