Variational method for the free-energy approximation of generalized anharmonic oscillators

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A variational method that uses the frequency and the energy shift as variational parameters is presented. The quantum-mechanical partition function is approximated by a formally simple expression, for a generalized anharmonic oscillator in one and many dimensions. The numerical calculations for a single quartic and two coupled quartic oscillators lead to nearly exact values for the free energy, the ground state, and the difference between the ground state and the first excited state.

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I. INTRODUCTION

Problems in quantum field theory, solid-state physics, and molecular vibrational motions theory have led to the investigation of the thermodynamic properties of various nonlinear systems [1–3]. Also anharmonic oscillators (AHO) have been used as testing examples for new methods in the above theories [4,5]. The present investigation is mainly concerned with the determination of the partition function (PF).

Apart from the calculation of energy eigenvalues, which presents a lot of difficulties, especially in the multidimensional case, several other methods have been developed for the approximation of the partition function of AHO's.

The thermodynamic perturbation method, which is based on perturbation treatment of the canonical density matrix [6], is easily applied up to second-order terms with respect to the anharmonic coupling and with some difficulty up to fourth-order terms [7,8]. The disadvantage here is that the results are only valid for quite small coupling. This disadvantage can be overcome by the use of variational methods.

Witschel and Bohmann [3] modified the Hamiltonian of the quartic AHO so that the frequency can be used as a variational parameter. Thus they succeeded in improving the lower and upper bounds of the PF in comparison to those obtained from Gibbs-Bogoliubov and Golden-Thompson inequalities [10].

Some time ago, Feynman and Kleinert [11] presented another method where, by the use of path-integral formulation, the PF can be approximated from below by an effective classical PF. This method was applied to the quartic and the double-well AHO's with nearly exact results. However, its extension to many-particle systems seems to be somewhat complicated.

For this reason Büttner and Flytzanis [12] suggested another method which includes both frequency and displacement as variational parameters. Its application for the above potentials is easier to use but leads to less exact results than the Feynman-Kleinert results. Nevertheless, in the zero-temperature limit both methods give the same value for the ground state.

Recently Kleinert, as well as Haugerud and Ravndal [13], proved that the finite-temperature Gaussian effective potential [14] is an upper limit to the free energy for a scalar quantum field theory. The application of this method to the field theory in zero spatial dimensions gives results similar to those in Ref. [12].

In this work we generalize the Gibbs-Bogoliubov variational principle [10] by introducing an energy shift variational parameter (Sec. II). In Sec. III we also use the frequency as variational parameter and using the results of Ref. [8] we find an approximation, in a simple form, for the PF of a generalized one-dimensional AHO. The application to quartic AHO's gives good results for the free energy, the ground state, and the difference between ground and first excited states (Sec. IV). Finally, in Sec. V, we extend this formalism to a multi-dimensional system with application to two coupled AHO's. In all these applications we have used natural units where $\hbar=c=1$ and therefore energy, mass, inverse length, and inverse time have the same dimensions.

II. GENERALIZATION OF THE GIBBS-BOGOLIUBOV VARIATIONAL PRINCIPLE

To achieve an approximation of the PF where the energy shift is included as a variational parameter, we appropriately generalize the procedure which leads to the proof [10] of the Gibbs-Bogoliubov variational principle.

We define the function

$$Z(\epsilon)=\mathrm{Tr}e^{-\beta[H_1+\sigma I+\epsilon(H_2-\sigma I)]}, \tag{2.1}$$

where ϵ and σ are real parameters, I is the unit operator, β is the inverse temperature, and H_1 and H_2 are Hermitian operators, the sum of which gives the Hamiltonian of the system, i.e.,

$$H=H_1+H_2 , \tag{2.2}$$

so the PF is taken from Eq. (2.1) with the substitution $\epsilon=1$.

The Taylor expansion (with remainder) of the $Z(\epsilon)$ function about $\epsilon=0$ is written

$$Z(\epsilon)=\sum_{\kappa=0}^{v}\frac{\epsilon^\kappa}{\kappa!}\frac{d^\kappa}{d\epsilon^\kappa}Z(0)+\frac{\epsilon^{v+1}}{(v+1)!}\frac{d^{v+1}}{d\epsilon^{v+1}}Z(\epsilon') , \tag{2.3}$$

where $0\le\epsilon'\le\epsilon$. The $(v+1)$ derivative can be determined according to the relation [15]

$$\frac{d^{v+1}}{d\epsilon^{v+1}}Z(\epsilon)=v!\int_0^1 t_1^{v-1}dt_1\cdots\int_0^1 dt_v \mathrm{Tr}\left\{Be^{A+\epsilon B}\prod_{j=1}^{v}e^{-t_1\cdots t_j(A+\epsilon B)}Be^{t_1\cdots t_j(A+\epsilon B)}\right\}, \tag{2.4}$$

where we have set

$$A=-\beta(H_1+\sigma I) \quad \text{and} \quad B=-\beta(H_2-\sigma I)\ . \tag{2.5}$$

The elimination of the remainder term and the substitution $\epsilon=1$ in Eq. (2.3) lead to the determination of an approximate expression of the PF, i.e.,

$$Z_\mu(1)=\mathrm{Tr}e^{A}+\mathrm{Tr}\{Be^{A}\}+\sum_{\kappa=1}^{\mu}\frac{1}{\kappa+1}\mathrm{Tr}\int_0^1 t_1^{\kappa-1}dt_1\cdots\int_0^1 dt_\kappa\left\{Be^{A}\prod_{j=1}^{\kappa}e^{-t_1\cdots t_jA}Be^{t_1\cdots t_jA}\right\}, \tag{2.6}$$

with $\mu=1,2,\ldots$.

The most proper value for the σ parameter is found from the solution of the equation

$$\frac{\partial}{\partial\sigma}Z_\mu(1)=0 \tag{2.7}$$

which is the necessary condition for the maximization or for the minimization of the $Z_\mu(1)$ function.

In Appendix A we prove that the above condition is equivalent to the equation

$$\mathrm{Tr}\int_0^1 t_1^{\mu-1}dt_1\cdots\int_0^1 dt_\mu\left\{Be^{A}\prod_{j=1}^{\mu}e^{-t_1\cdots t_jA}\times Be^{t_1\cdots t_jA}\right\}=0\ . \tag{2.8}$$

This result is obtained by noting that on setting the last term of the sum in Eq. (2.6) equal to zero, condition (2.7) is automatically satisfied.

The above method can be regarded as a generalization of the Gibbs-Bogoliubov variational principle. In fact, if we keep the first two terms in the second part of Eq. (2.6) then the σ parameter, which is obtained from Eq. (2.7), has the form

$$\sigma=\frac{\mathrm{Tr}\{H_2\exp(-\beta H_1)\}}{\mathrm{Tr}\{\exp(-\beta H_1)\}} \tag{2.9}$$

and therefore Eq. (2.6) gives

$$Z_{\mathrm{LB}}=\mathrm{Tr}e^{-\beta H_1-\beta\sigma}\ , \tag{2.10}$$

which is the well-known Gibbs-Bogoliubov lower bound of the partition function.

III. ONE-DIMENSIONAL AHO

Following the idea of using frequency as a variational parameter [16,17] we can drastically improve the results of the preceding section.

Consider Eq. (2.6), up to fourth-order terms ($\mu=2$), with the following Hamiltonian:

$$H=\frac{p^2}{2}+\frac{\omega^2}{2}x^2+V(x)\ . \tag{3.1}$$

In this case we have

$$A=-\beta(H_0+\sigma) \quad \text{and} \quad B=-\beta\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right], \tag{3.2}$$

where

$$H_0=\frac{p^2}{2}+\frac{\omega_0^2}{2}x^2 \tag{3.3}$$

and

$$\Delta^2=\omega^2-\omega_0^2\ . \tag{3.4}$$

Keeping up to fourth-order terms ($\mu=2$) in the expansion of (2.6) we obtain the following expression of the PF for $\epsilon=1$:

$$\begin{aligned}Z_2=e^{-\beta\sigma}\Bigg\{&\mathrm{Tr}e^{-\beta H_0}-\beta\,\mathrm{Tr}\left[\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right]e^{-\beta H_0}\right]\\&+\frac{\beta^2}{2}\mathrm{Tr}\int_0^1 dt_1\left[\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right]e^{-\beta H_0}e^{\beta t_1H_0}\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right]e^{-\beta t_1H_0}\right]\\&-\frac{\beta^3}{3}\mathrm{Tr}\int_0^1 t_1dt_1\int_0^1 dt_2\left[\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right]e^{-\beta H_0}e^{\beta t_1H_0}\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right]\right.\\&\left.\times e^{-\beta t_1H_0}e^{\beta t_1t_2H_0}\left[\frac{\Delta^2}{2}x^2+V(x)-\sigma\right]e^{-\beta t_1t_2H_0}\right]\Bigg\}.\end{aligned} \tag{3.5}$$

This expression depends on two variational parameters, namely, the energy shift σ and the frequency ω_0. The optimum values of σ and ω_0 are determined from the solution of the system

$$\frac{\partial Z_2}{\partial \sigma}=0, \quad \frac{\partial Z_2}{\partial \omega_0}=0 . \tag{3.6}$$

In order to proceed, we put the expressions of Eq. (3.5) in a more convenient form. To this end we make use of the following relations [8]:

$$\mathrm{Tr}(x^{\rho}e^{-\beta H_0}e^{\beta t_1 H_0}x^{\kappa}e^{-\beta t_1 H_0})=Z_0\mathcal{L}^{\rho\kappa}(t_1;\beta,\omega_0) , \tag{3.7}$$

$$\mathrm{Tr}(x^{\rho}e^{-\beta H_0}e^{\beta t_1 H_0}x^{\kappa}e^{-\beta t_1(1-t_2)H_0}x^{\tau}e^{-\beta t_1 t_2 H_0})=Z_0\mathcal{L}^{\rho\kappa\tau}(t_1,t_2;\beta,\omega_0) , \tag{3.8}$$

where

$$Z_0=\frac{1}{2\sinh(\beta\omega_0/2)} \tag{3.9}$$

is the PF which corresponds to the Hamiltonian H_0 and

$$\mathcal{L}^{\rho\kappa}(t_1;\beta,\omega_0)=\kappa!\left[\frac{1}{2\omega_0}\coth\frac{\beta\omega_0}{2}\right]^{(\rho+\kappa)/2}A_1^{\kappa}\sum_{s=0}^{[\kappa/2]}\frac{(\rho+\kappa-2s-1)!!}{2^s s!(\kappa-2s)!}\left[\frac{1-A_1^2}{A_1^2}\right]^s , \tag{3.10}$$

$$\mathcal{L}^{\rho\kappa\tau}(t_1,t_2;\beta,\omega_0)=\kappa!\tau!\left[\frac{1}{2\omega_0}\coth\frac{\beta\omega_0}{2}\right]^{(\rho+\kappa+\tau)/2}A_1^{\tau}A_2^{\kappa}\times\sum_{s_2=0}^{[\kappa/2]}\sum_{s_1=0}^{[\tau/2]}\sum_{l_1=0}^{\kappa-2s_2}\frac{[\rho+\kappa+\tau-2(s_1+s_2)-2l_1-1]!!}{2^{s_1+s_2}s_1!s_2!l_1!(\kappa-2s_2-l_1)!(\tau-2s_1-l_1)!}\times\left[\frac{1-A_1^2}{A_1^2}\right]^{s_1}\left[\frac{1-A_2^2}{A_2^2}\right]^{s_2}\left[\frac{A_{12}-A_1A_2}{A_1A_2}\right]^{l_1} , \tag{3.11}$$

with $\tau-2s_1-l_1\geq 0$ $[\alpha]$ the integral part of the real number α and

$$A_1=\frac{\cosh[(\beta\omega_0/2)(1-2t_1)]}{\cosh(\beta\omega_0/2)} ,$$

$$A_2=\frac{\cosh[(\beta\omega_0/2)(1-2t_1t_2)]}{\cosh(\beta\omega_0/2)} , \tag{3.12}$$

$$A_{12}=\frac{\cosh[(\beta\omega_0/2)(1-2t_1+2t_1t_2)]}{\cosh(\beta\omega_0/2)} .$$

We complete the above with the definitions

$$\mathcal{L}^0=1 ,$$

$$\mathcal{L}^{\kappa}(\beta,\omega_0)=(\kappa-1)!!\left[\frac{1}{2\omega_0}\coth\frac{\beta\omega_0}{2}\right]^{\kappa/2} . \tag{3.13}$$

Some useful properties of the above-defined $\mathcal{L}$ functions are

$$\int_0^1 dt_1\mathcal{L}^{\rho\kappa}(t_1;\beta,\omega_0)=\int_0^1 dt_1\mathcal{L}^{\kappa\rho}(t_1;\beta,\omega_0) , \tag{3.14}$$

which is a result of the trace cyclic property. Also the quantity

$$\int_0^1 t_1dt_1\int_0^1 dt_2\mathcal{L}^{\rho\kappa\tau}(t_1,t_2;\beta,\omega_0) \tag{3.15}$$

is invariant with respect to permutations of ρ,κ,τ (see Appendix B).

If the potential $V(x)$ admits the expansion

$$V(x)=\sum_{\kappa}c_{\kappa}x^{\kappa} \tag{3.16}$$

then using the properties in Eqs. (3.14) and (3.15) and the traces (3.7) and (3.8) appearing in Eq. (3.5), we can present the approximation of the PF in the following formally simple expression:

$$Z_2=e^{-\beta\sigma}Z_0\left\{1-\beta Q(\sigma,\omega_0)+\frac{\beta^2}{2}\int_0^1 dt_1Q^2(\sigma,\omega_0)-\frac{\beta^3}{3}\int_0^1 t_1dt_1\int_0^1 dt_2Q^3(\sigma,\omega_0)\right\} , \tag{3.17}$$

where

$$Q(\sigma,\omega_0)=\frac{\Delta^2}{2}\mathcal{L}^2+V(\mathcal{L})-\sigma\mathcal{L}^0 \tag{3.18}$$

and the Q^2 and Q^3 functions are calculated with the understanding that the multiplication of $\mathcal{L}$ is done with the following rules:

$$\mathcal{L}^{\rho}\mathcal{L}^{\kappa}=\mathcal{L}^{\rho\kappa} ,$$

$$\mathcal{L}^{\rho\kappa}\mathcal{L}^{\tau}=\mathcal{L}^{\rho\kappa\tau} . \tag{3.19}$$

Finally Eqs. (3.6) take the form

$$\int_0^1 t_1dt_1\int_0^1 dt_2Q^3(\sigma,\omega_0)=0 , \tag{3.20}$$

$$\frac{\beta}{2}\coth\frac{\beta\omega_0}{2}=\frac{\partial}{\partial\omega_0}\ln\left\{1-\beta Q+\frac{\beta^2}{2}\int_0^1 dt_1Q^2-\frac{\beta^3}{3}\int_0^1 t_1dt_1\int_0^1 dt_2Q^3\right\} \tag{3.21}$$

and the solution of this system gives the optimum pair of (σ,ω_0) for each value of β.

We apply the above method to a quartic AHO, with Hamiltonian $H=p^2/2+x^2/2+\lambda x^4$, for relatively small ($\lambda=1$) and large ($\lambda=10$) anharmonic coupling and we find that the resulting PF is a lower bound of the exact

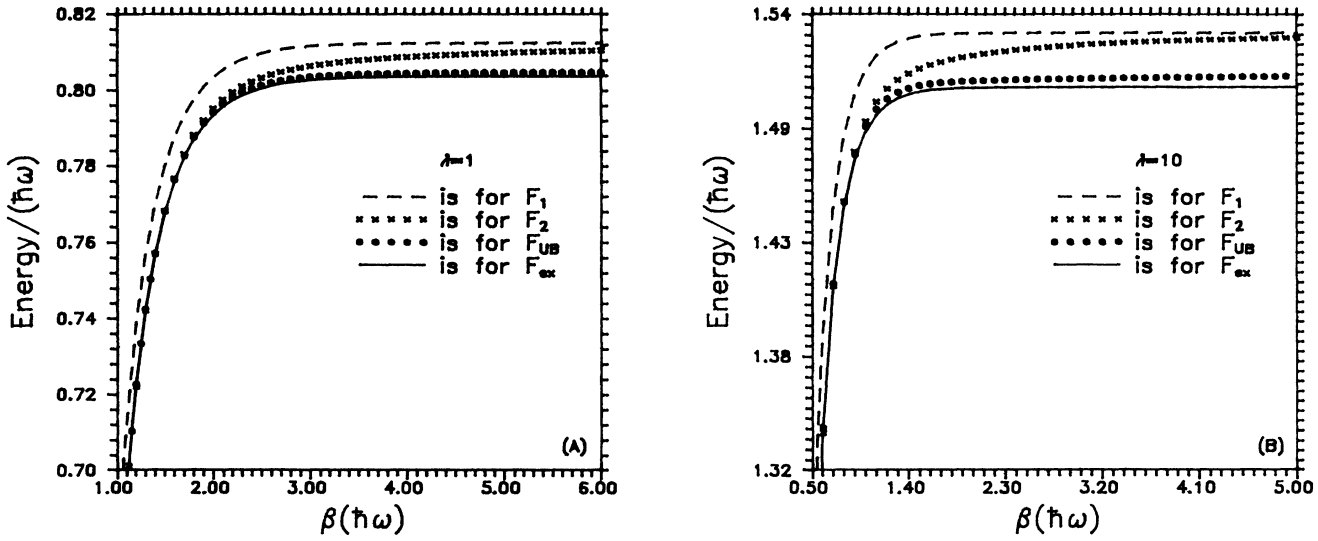

FIG. 1. Inverse temperature (β) dependence of the approximate free energies F_1, F_2, and $F_{\rm UB}$, for the AHO with Hamiltonian $H=p^2/2+x^2/2+\lambda x^4$ in the cases (a) $\lambda=1$ and (b) $\lambda=10$ and the exact free energy $F_{\rm ex}$ (Ref. [18]).

one [18]. The corresponding free-energy upper bound $F_{\rm UB}=-(1/\beta)\ln(Z_2)$ is drawn in Figs. 1(a) and 1(b), for the above values of λ, respectively, and is compared with the exact [18] free energy $F_{\rm ex}$, the Feynman-Kleinert F_1, and the free energy F_2 resulting from Refs. [9,12,13]. The values of the approximate free energy F_2 can be obtained from the above method, if we keep the first two terms in the sum of Eq. (3.5) (first approximation).

We observe that except to very large temperatures, the $F_{\rm UB}$ function approaches much better the exact curve than the F_1 function, while F_2 lies far above both of them. We notice also that the difference between $F_{\rm UB}$ and $F_{\rm ex}$ is small in the case of $\lambda=1$ and becomes larger when $\lambda=10$.

IV. GROUND-STATE ENERGY

It is well known that the ground-state energy is given by the zero-temperature limit (ZTL) of the free energy F or of the internal energy U. We consider the Hamiltonian of the preceding section and the expression (2.6) for the PF. We can obtain the ground-state energy from the ZTL of the following relation:

$$U=\frac{d}{d\beta}(\beta F)\ , \tag{4.1}$$

which, taking into account the conditions

$$\frac{\partial}{\partial\sigma}Z_\mu(1)=0,\quad \frac{\partial}{\partial\omega_0}Z_\mu(1)=0\ , \tag{4.2}$$

can be written in the form

$$\frac{d}{d\beta}(\beta F)=-\frac{1}{Z_0}\frac{\partial Z_0}{\partial\beta}-\frac{1}{Z_I}\frac{\partial Z_I}{\partial\beta}\ . \tag{4.3}$$

Here

$$Z_0=\frac{e^{-\beta\sigma}}{2\sinh(\beta\omega_0/2)}\ , \tag{4.4}$$

$$Z_I=1-\beta\frac{\mathrm{Tr}[W(x)e^{-\beta H_0}]}{\mathrm{Tr}e^{-\beta H_0}}+\sum_{\kappa=1}^{\mu}\frac{\beta^{\kappa+1}}{\kappa+1}\frac{\mathrm{Tr}\int_0^1 t_1^{\kappa-1}dt_1\cdots\int_0^1 dt_\kappa\left\{W(x)e^{-\beta H_0}\prod_{j=1}^{\kappa}e^{\beta t_1\cdots t_j H_0}W(x)e^{-\beta t_1\cdots t_j H_0}\right\}}{\mathrm{Tr}e^{-\beta H_0}}\ , \tag{4.5}$$

and

$$W(x)=\frac{\Delta^2}{2}x^2+V(x)-\sigma\ . \tag{4.6}$$

It is straightforward to show directly from Eqs. (C1) and (C3) that

$$\lim_{\beta\to\infty}\frac{1}{Z_I}\frac{\partial Z_I}{\partial\beta}=0\ . \tag{4.7}$$

Therefore the ZTL of the internal energy gives

$$E_1^0=\lim_{\beta\to\infty} U=\frac{\omega_0}{2}+\sigma \ , \tag{4.8}$$

where the optimum pair (σ,ω_0) is defined by the relations

$$\sigma=\frac{\Delta^2}{4\omega_0}+\sum_\kappa c_\kappa(\kappa-1)!!\left[\frac{1}{2\omega_0}\right]^{\kappa/2} , \tag{4.9}$$

$$\frac{\Delta^2}{4\omega_0}+\sum_\kappa c_\kappa(\kappa-1)!!\frac{\kappa}{2}\left[\frac{1}{2\omega_0}\right]^{\kappa/2}=0 , \tag{4.10}$$

which follow from the ZTL of Eqs. (4.2). Finally, by combining Eqs. (4.8) and (4.9) we obtain

$$E_1^0=\frac{\omega_0}{2}+\frac{\Delta^2}{4\omega_0}+\sum_\kappa c_\kappa(\kappa-1)!!\left[\frac{1}{2\omega_0}\right]^{\kappa/2} . \tag{4.11}$$

An identical result for E_1^0 can be reached by taking the ZTL of the free energy

$$F=-\frac{1}{\beta}\ln Z_0-\frac{1}{\beta}\ln Z_I \ . \tag{4.12}$$

In fact, assuming that the limit appearing in Eq. (C1) can be applied separately to each term of the series in Eq. (4.5) we may write the following equality:

$$\lim_{\beta\to\infty} Z_I=\lim_{\beta\to\infty}\exp\left\{-\beta\left[\frac{\Delta^2}{4\omega_0}+\sum_\kappa c_\kappa(\kappa-1)!!\times\left[\frac{1}{2\omega_0}\right]^{\kappa/2}-\sigma\right]\right\} . \tag{4.13}$$

Accordingly the ZTL of Eq. (4.12) easily leads to Eq. (4.11).

The approximation E_1^0 to the ground-state energy as it is given by Eq. (4.11) can also be obtained from the minimal expectation value of the operator (3.1), with the condition (3.16), in a Gaussian wave packet of the form $(\omega_0/\pi)^{1/4}\exp(-\omega_0 x^2/2)$. The condition for ω_0 to minimize this expectation value is found to be identical to Eq. (4.10). The above wave packet has been used by Feynman and Kleinert [11]. In the case of quartic AHO, the Ω parameter of Ref. [11] corresponds to the ω_0 of the present work since both parameters satisfy the same equation, namely, Eq. (4.10) with $\kappa=4$.

To go beyond the $\beta\to\infty$ approximation described above, we consider Fig. 1 from which it is evident that the value of the $F_{\rm UB}$ free energy of the quartic AHO nearly coincides with the exact value of the free energy in a fairly wide range of intermediate temperatures. It will be shown that we can much better approximate the ground state by exploiting this fact.

In Fig. 2 we have drawn the curves for (i) the $F_{\rm UB}$ free energy and the internal energy U obtained from $F_{\rm UB}$ (both $F_{\rm UB}$ and U tend to the common limit E_1^0) and (ii) the corresponding exact functions $F_{\rm ex}$ and $U_{\rm ex}$ which have as common limit the exact ground state $E_{\rm ex}^0$.

As we know, the internal energy is a decreasing function with respect to β, and should be larger than the free energy which is an increasing function with respect to β. However, from Fig. 2 we may conclude that the U function does not follow the above behavior because it has a minimum at a certain value β_0 of the variable β. This happens because $F_{\rm UB}$ is a very good approximation of the $F_{\rm ex}$ when $\beta<\beta_0$ so that the corresponding U function agrees quite well with $U_{\rm ex}$ until the value β_0 is reached. Also β_0 is in a range of small temperatures where $F_{\rm ex}$ has approached $E_{\rm ex}^0$. From the above consideration we can conclude that the value

$$E^0=F_{\rm UB}(\beta_0) \tag{4.14}$$

gives a better estimate of the ground state than the E_1^0.

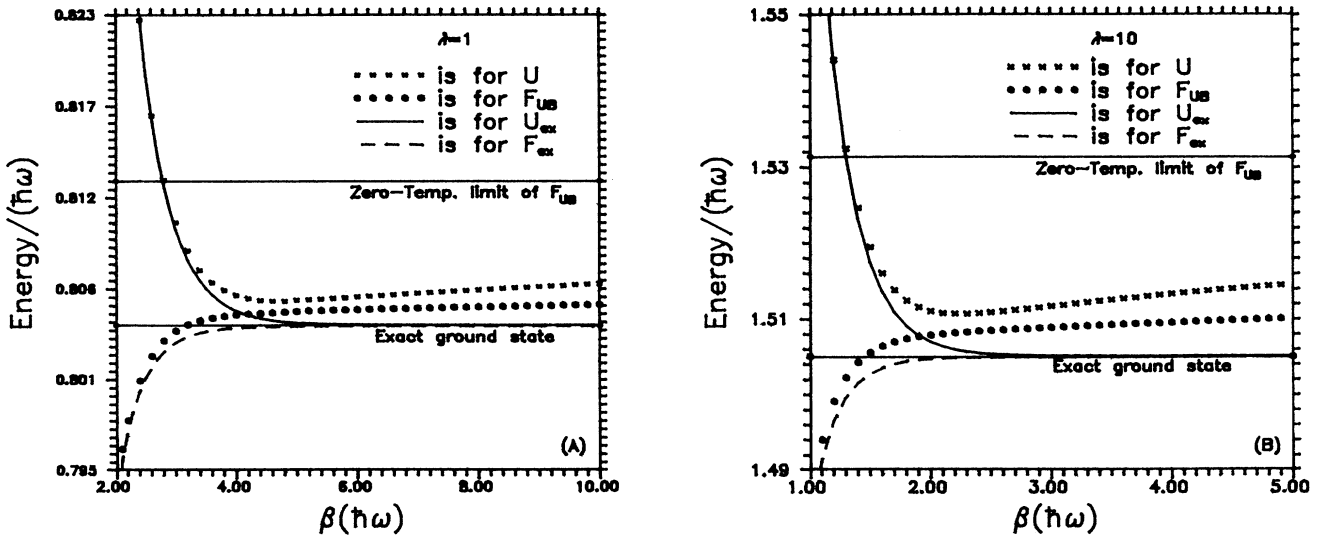

FIG. 2. Dependence on β of the exact ($F_{\rm ex}$) and approximate ($F_{\rm UB}$) free energy and the corresponding internal energies ($U_{\rm ex}$, U), for the AHO of Fig. 1. Note that the approximate internal energy has a minimum in the range between the exact ground state and the zero-temperature limit of $F_{\rm UB}$.

TABLE I. Comparison of $E^0=F_{UB}(\beta_0)$ with the exact ground-state value E^0_{ex} (in parentheses) and also of the difference from the first excited state [18] $E^1_{ex}-E^0_{ex}$ (in parentheses) with $\sigma+\omega_0$ evaluated at β_0.

λ	E^0	(E^0_{ex})	$\sigma+\omega_0$	$(E^1_{ex}-E^0_{ex})$	β_0
0.5	0.696 62	(0.696 18)	1.618 33	(1.628 23)	6.0
1.0	0.804 62	(0.803 77)	1.921 74	(1.934 12)	4.8
10.0	1.508 15	(1.504 97)	3.790 87	(3.816 94)	2.2
1000.0	6.712 17	(6.694 22)	17.147 41	(17.278 00)	0.5

Noting that at the limit $\beta\to\infty$ the ω_0 parameter gives the difference between the ground and the first excited state [11], we have a substantial improvement of the difference if we add to the ω_0 the σ parameter as evaluated at $\beta=\beta_0$. Energy values obtained in this way are listed in Table I and are compared with the corresponding exact energies in a wide range of anharmonic coupling values.

We observe that the accuracy for the ground state and the difference between the ground and first excited states is quite satisfactory for small coupling and remains reasonable for large coupling.

V. MULTIDIMENSIONAL AHO

The formalism of the third section can be explained to multidimensional systems which have the Hamiltonian

$$H=\sum_{i=1}^{D} H_{0i}+V(x_1,x_2,\ldots,x_D)\ , \tag{5.1}$$

where

$$H_{0i}=\frac{p^2}{2}+\frac{\omega_i^2}{2}x_i^2 \tag{5.2}$$

and $V(x_1,x_2,\ldots,x_D)$ is a function which admits the expansion

$$V(x_1,x_2,\ldots,x_D)=\sum_{\kappa_1,\ldots,\kappa_D} c_{\kappa_1\kappa_2\cdots\kappa_D}x_1^{\kappa_1}x_2^{\kappa_2}\cdots x_D^{\kappa_D}\ , \tag{5.3}$$

with $c_{\kappa_1\kappa_2\cdots\kappa_D}$ constant coefficients.

Here we introduce the energy shift σ and D frequency variational parameters $\omega_{01},\ldots,\omega_{0D}$, one for each particle.

Following the steps of Sec. III we define

$$\begin{aligned} A&=-\beta\sum_{i=1}^{D}(H_{0i}+\sigma)\ ,\\ B&=-\beta\left\{\sum_{i=1}^{D}\frac{\Delta_i^2}{2}x_i^2+\beta V(x_1,x_2,\ldots,x_D)-D\sigma\right\}\ , \end{aligned} \tag{5.4}$$

where $\Delta_i^2=\omega_i^2-\omega_{0i}^2$ and after analogous manipulation we find that

$$\begin{aligned} Z_2=Z_0\Big\{&1-\beta Q(\sigma,\omega_{01},\ldots,\omega_{0D})\\ &+\frac{\beta^2}{2}\int_0^1 dt_1 Q^2(\sigma,\omega_{01},\ldots,\omega_{0D})\\ &-\frac{\beta^3}{3}\int_0^1 t_1dt_1\int_0^1 dt_2 Q^3(\sigma,\omega_{01},\ldots,\omega_{0D})\Big\}\ , \end{aligned} \tag{5.5}$$

where

$$Z_0=\frac{e^{-\beta D\sigma}}{2^D\sinh(\beta\omega_{01}/2)\cdots\sinh(\beta\omega_{0D}/2)} \tag{5.6}$$

and

$$\begin{aligned} Q(\sigma,\omega_{01},\ldots,\omega_{0D})=&\sum_{i=1}^{D}\frac{\Delta_i^2}{2}\mathcal{L}_1^0\cdots\mathcal{L}_i^2\cdots\mathcal{L}_D^0\\ &+V(\mathcal{L}_1,\ldots,\mathcal{L}_D)-\sigma D\mathcal{L}_1^0\cdots\mathcal{L}_D^0\ . \end{aligned} \tag{5.7}$$

Here we have to clarify the symbolism. The subscript of the function $\mathcal{L}$ is a particle index. The product of such functions is defined according to the rule (3.19) when they are associated with a single particle, while for different particles the product is the usual one. Finally, the system which determines the values of the variational parameters now has the form

$$\begin{aligned} &\int_0^1 t_1dt_1\int_0^1 dt_2Q^3(\sigma,\omega_{01},\ldots,\omega_{0D})=0\ ,\\ &\frac{\beta}{2}\coth\frac{\beta\omega_{0i}}{2}=\frac{\partial}{\partial\omega_{0i}}\ln\left\{1-\beta Q+\frac{\beta^2}{2}\int_0^1 dt_1Q^2\right.\\ &\qquad\left.-\frac{\beta^3}{3}\int_0^1 t_1dt_1\int_0^1 dt_2Q^3\right\}\ , \end{aligned} \tag{5.8}$$

with $i=1,2,\ldots,D$.

We apply this method in two coupled AHO's with Hamiltonian

$$H=\frac{p_1^2}{2}+\frac{p_2^2}{2}+\frac{x_1^2}{2}+\frac{x_2^2}{2}+gx_1^4+g_{12}x_1^2x_2^2+gx_2^4 \tag{5.9}$$

for several values of g and g_{12}. The resulting curves for free and internal energy for these systems are similar to the ones in Figs. 1 and 2. The ground state E^0_α, as obtained by full application of the above method and the ground state E^0_b, as obtained by the first approximation,

TABLE II. Comparison of E_a^0 and E_b^0 with E_{ex}^0 and also of the difference from the first excited state [18] $E_{ex}^1 - E_{ex}^0$ (in parentheses) with $\sigma+\omega_0$ evaluated at β_0.

g	g_{12}	E_a^0	E_b^0	E_{ex}^0	$\sigma+\omega_0$	$(E_{ex}^1 - E_{ex}^0)$	β_0
1	0.4	1.6496	1.6362	1.6332	1.9169	(1.9741)	5.1
1	2.0	1.7401	1.7305	1.7242	1.9985	(2.1062)	4.8
100	120	6.7778	6.7101	6.6741	8.2114	(8.6409)	1.1

are presented in Table II. These values as well as the difference between the ground state and the first excited state $(\sigma+\omega_0)$ are compared with the exact results [18] and one can observe that the results here are less accurate than in the one-dimensional case, especially for large values of g and g_{12}.

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APPENDIX A

We will here prove, by induction, that

$$\frac{\partial}{\partial\sigma}Z_\mu(1) = -\frac{\beta}{\mu+1}\mathrm{Tr}\int_0^1 t_1^{\mu-1}dt_1\cdots\int_0^1 dt_\mu\left\{Be^{A}\prod_{j=1}^{\mu}e^{-t_1\cdots t_jA}Be^{t_1\cdots t_jA}\right\}, \tag{A1}$$

with $\mu=1,2,3,\ldots$. For $\mu=1$ Eq. (2.6) is written

$$\frac{\partial}{\partial\sigma}Z_1 = -\frac{\beta}{2}\mathrm{Tr}\{Be^{A}\} + \frac{\beta}{2}\mathrm{Tr}\int_0^1 dt_1 e^{A}e^{-t_1A}Be^{t_1A} - \frac{\beta}{2}\mathrm{Tr}\int_0^1 dt_1 Be^{A}e^{-t_1A}Be^{t_1A}, \tag{A2}$$

which due to the relations

$$\mathrm{Tr}\left\{\frac{\partial}{\partial\epsilon}e^{A+\epsilon B}\right\}_{\epsilon=0} = \mathrm{Tr}\{Be^{A}\} = \mathrm{Tr}\int_0^1 dt_1 e^{A}e^{-t_1A}Be^{t_1A} \tag{A3}$$

finally gives

$$\frac{\partial}{\partial\sigma}Z_1 = -\frac{\beta}{2}\mathrm{Tr}\int_0^1 dt_1 Be^{A}e^{-t_1A}Be^{t_1A} \tag{A4}$$

so Eq. (A1) is valid for $\mu=1$.

We suppose now that Eq. (A1) is valid and we shall prove its validity for $\mu+1$. It follows from Eq. (2.6) that

$$\frac{\partial}{\partial\sigma}Z_{\mu+1} = \frac{\partial}{\partial\sigma}Z_\mu + \frac{1}{\mu+2}\mathrm{Tr}\int_0^1 t_1^{\mu}dt_1\cdots\int_0^1 dt_{\mu+1}\frac{\partial}{\partial\sigma}\left\{Be^{A}\prod_{j=1}^{\mu+1}e^{-t_1\cdots t_jA}Be^{t_1\cdots t_jA}\right\} \tag{A5}$$

and therefore by carrying out the σ derivative we end up with

$$\begin{aligned}\frac{\partial}{\partial\sigma}Z_{\mu+1} = &-\frac{\beta}{\mu+2}\mathrm{Tr}\int_0^1 t_1^{\mu}dt_1\cdots\int_0^1 dt_{\mu+1}Be^{A}\prod_{j=1}^{\mu+1}e^{-t_1\cdots t_jA}Be^{t_1\cdots t_jA}\\ &+\beta\mathrm{Tr}\int_0^1 t_1^{\mu}dt_1\cdots\int_0^1 dt_{\mu+1}e^{A}\prod_{j=1}^{\mu+1}e^{-t_1\cdots t_jA}Be^{t_1\cdots t_jA}\\ &-\frac{\beta}{\mu+1}\mathrm{Tr}\int_0^1 t_1^{\mu-1}dt_1\cdots\int_0^1 dt_\mu Be^{A}\prod_{j=1}^{\mu}e^{-t_1\cdots t_jA}Be^{t_1\cdots t_jA}.\end{aligned} \tag{A6}$$

On the other hand, the substitution of the derivatives (2.4) in the following obvious relation:

$$\mathrm{Tr}\left\{\frac{\partial^{\mu+1}}{\partial\epsilon^{\mu+1}}e^{A+\epsilon B}\right\}_{\epsilon=0} = \mathrm{Tr}\left\{B\frac{\partial^{\mu}}{\partial\epsilon^{\mu}}e^{A+\epsilon B}\right\}_{\epsilon=0} \tag{A7}$$

leads to the cancellation of the last two terms in Eq. (A6). Thus Eq. (A1) is also valid for $\mu+1$.

APPENDIX B

The property (3.15) is proved as follows. Let A, B_1, B_2, and B_3 be Hermitian operators. Using the transformations

$$
\begin{aligned}
&t_1=T_1,\quad t_2=1-T_2\ ,\\
&t_1=1-T_1T_2,\quad t_1t_2=T_1-T_1T_2\ ,\\
&t_1=1-T_1T_2,\quad t_1t_2=1-T_1\ ,\\
&t_1=1-T_1+T_1T_2,\quad t_1t_2=1-T_1\ ,\\
&t_1=1-T_1+T_1T_2,\quad t_1t_2=T_1T_2\ ,
\end{aligned}
\tag{B1}
$$

and the trace cyclic property, we can easily prove that the integral

$$
\int_0^1 t_1dt_1\int_0^1 dt_2\mathrm{Tr}\left\{B_1e^{-(1-t_1)A}B_2\times e^{-(t_1-t_1t_2)A}B_3e^{-t_1t_2A}\right\} \tag{B2}
$$

is invariant for all permutations of the operators

$$
e^{-(1-t_1)A},\quad e^{-(t_1-t_1t_2)A},\quad e^{-t_1t_2A}
$$

as well as for cyclic permutations of the B_1,B_2,B_3.

It will be proven that, in the case where

$$
\begin{aligned}
&A=\beta\left[\frac{p^2}{2}+\frac{\omega^2}{2}x^2\right]=\beta H_0\ ,\\
&B_1=x^\rho,\quad B_2=x^\kappa,\quad B_3=x^\tau
\end{aligned}
\tag{B3}
$$

the resulting integral (B2) is also invariant for all permutations of x^ρ, x^κ, and x^τ. In fact, using the coordinate representation the integrand of (B2) takes the form

$$
\begin{aligned}
&\mathrm{Tr}(x^\rho e^{-\beta(1-t_1)H_0}x^\kappa e^{-\beta(t_1-t_1t_2)H_0}x^\tau e^{-\beta t_1t_2H_0})\\
&\quad=\int_{-\infty}^{\infty}dx\,dx_1dx_2[x^\rho\rho_0(x,x_1;\beta(1-t_1))x_1^\kappa\rho_0(x_1,x_2;\beta(t_1-t_1t_2))x_2^\tau\rho_0(x_2,x;\beta t_1t_2)]\ ,
\end{aligned}
\tag{B4}
$$

where ρ_0 is the well-known density matrix which corresponds to Hamiltonian H_0. Since the ρ_0 function is symmetric with respect to the coordinate variables, we can rewrite the above relation as

$$
\begin{aligned}
&\int_{-\infty}^{\infty}dx_1dx\,dx_2[x_1^\kappa\rho_0(x_1,x;\beta(1-t_1))x^\rho\rho_0(x,x_2;\beta t_1t_2))x_2^\tau\rho_0(x_2,x_1;\beta t_1(1-t_2))]\\
&\quad=\mathrm{Tr}(x^\kappa e^{-\beta(1-t_1)H_0}x^\rho e^{-\beta t_1t_2H_0}x^\tau e^{-\beta t_1(1-t_2)H_0})\ ,
\end{aligned}
\tag{B5}
$$

which proves the invariance with respect to permutation of x^ρ, x^κ, and x^τ.

APPENDIX C

We will prove the relation

$$
\lim_{\beta\to\infty}\frac{\mathrm{Tr}\left\{W(x)e^{-\beta H_0}\prod_{j=1}^{n}e^{\beta t_1\cdots t_jH_0}W(x)e^{-\beta t_1\cdots t_jH_0}\right\}}{\mathrm{Tr}e^{-\beta H_0}}=\left\{\sum_\kappa d_\kappa(\kappa-1)!!\left[\frac{1}{2\omega}\right]^{\kappa/2}\right\}^{n+1}\ , \tag{C1}
$$

where κ is an even integer,

$$
H_0=\frac{p^2}{2}+\frac{\omega^2}{2}x^2,\quad\text{and}\quad W(x)=\sum_\kappa d_\kappa x^\kappa\ , \tag{C2}
$$

with d_κ constant coefficients.

Expanding the $W(x)$ functions according to Eq. (C2), we can write the first term of Eq. (C1) as follows [8,19]:

$$
\begin{aligned}
&\lim_{\beta\to\infty}\left[\frac{\omega}{\pi\coth(\beta\omega/2)}\right]^{1/2}\sum_{\kappa_0}\cdots\sum_{\kappa_n}d_{\kappa_0}\cdots d_{\kappa_n}\left[\frac{\sinh\beta\omega\xi_1}{\omega}\right]^{\kappa_1}\cdots\left[\frac{\sinh\beta\omega\xi_n}{\omega}\right]^{\kappa_n}\\
&\times\int_{-\infty}^{\infty}x^{\kappa_0}e^{-\omega\tanh(\beta\omega/2)x^2}\left\{\sum_{s_n=0}^{[\kappa_n/2]}\frac{\kappa_n!a_n^{s_n}}{2^{s_n}s_n!(\kappa_n-2s_n)!}\left[2Nx+a_nx_1+\frac{d}{dx_1}\right]_N^{\kappa_n-2s_n}\right.\\
&\left.\times\cdots\sum_{s_1=0}^{[\kappa_1/2]}\frac{\kappa_1!a_1^{s_1}}{2^{s_1}s_1!(\kappa_1-2s_1)!}\left[2Nx+a_1x_1+\frac{d}{dx_1}\right]_N^{\kappa_1-2s_1}1\right\}_{x=x_1}dx\ ,
\end{aligned}
\tag{C3}
$$

$$N=\frac{\omega}{2\sinh(\beta\omega)},\quad a_i=\frac{\omega\sinh[\beta\omega(1-\xi_i)]}{\sinh(\beta\omega)\sinh(\beta\omega\xi_i)},$$
$$\xi_i=t_1t_2\cdots t_i \qquad \text{(C4)}$$

and the symbol N denotes the normal ordering of operators [19]. Because the integral in expression (C3) is uniformly convergent (being a sum of Γ functions), we can take the limit of each factor in the integrand.

Thus the expression (C3) tends to the following limit:

$$\sum_{\kappa_0} d_{\kappa_0}\frac{(\kappa_0-1)!!}{(2\omega)^{\kappa_0/2}}\sum_{\kappa_1} d_{\kappa_1}\frac{\kappa_1!}{2^{\kappa_1/2}(\kappa_1/2)!}\left[\frac{1}{2\omega}\right]^{\kappa_1/2}\times\sum_{\kappa_n} d_{\kappa_n}\frac{\kappa_n!}{2^{\kappa_n/2}(\kappa_n/2)!}\left[\frac{1}{2\omega}\right]^{\kappa_n/2}, \qquad \text{(C5)}$$

when $\kappa_0,\kappa_1,\ldots,\kappa_n$ are even integers and zero when any of the κ's is an odd integer. It is now obvious that (C5) is identical to the second term of Eq. (C1).

[1] R. Giachetti and V. Tognetti, Phys. Rev. B **33**, 7647 (1986).
[2] R. Giachetti, V. Tognetti, and R. Vaia, Phys. Rev. A **37**, 2165 (1988).
[3] G. Vlastou-Tsinganos, N. Flytzanis, and H. Büttner, J. Phys. A **23**, 4553 (1990).
[4] A. Okopińska, Phys. Rev. D **35**, 1835 (1987); **36**, 2415 (1987).
[5] P. M. Stevenson, Phys. Rev. D **30**, 1712 (1984).
[6] G. V. Chester, Phys. Rev. **93**, 606 (1954); J. Schwinger, Phys. Rev. **82**, 664 (1951).
[7] C. E. Harvie, P. Bopp, and M. Wolfsberg, J. Chem. Phys. **72**, 6349 (1980).
[8] K. Vlachos, Phys. Lett. A **141**, 65 (1989).
[9] W. Witschel and J. Bohmann, J. Phys. A **13**, 2735 (1980).
[10] M. Girardeau and R. Mazo, Adv. Chem. Phys. **24**, 187 (1973).
[11] R. P. Feynman and H. Kleinert, Phys. Rev. A **34**, 5080 (1986).
[12] H. Büttner and N. Flytzanis, Phys. Rev. A **36**, 3443 (1987).
[13] H. Kleinert, Phys. Lett. A **118**, 195 (1986); H. Haugerud and F. Ravndal, Phys. Rev. D **43**, 2736 (1991).
[14] G. A. Hajj and P. M. Stevenson, Phys. Rev. D **37**, 413 (1988).
[15] K. Kumar, J. Math. Phys. **6**, 1928 (1965).
[16] W. E. Caswell, Ann. Phys. (N.Y.) **123**, 153 (1979).
[17] J. Killingbeck, J. Phys. A **14**, 1005 (1981).
[18] F. T. Hioe, D. MacMillen, and E. W. Montroll, Phys. Rep. **43**, 305 (1978).
[19] R. M. Wilcox, J. Math. Phys. **8**, 962 (1966).