Generalized anharmonic oscillator: A simple variational approach. II. The D-dimensional anisotropic case

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(Received 28 July 1981)

An approximate, variational method for the study of the generalized anharmonic oscillator in D dimensions is given, where the anharmonicity is represented by a broad class of even functions of the D coordinates. The idea of the method is to introduce into the unperturbed oscillator states the correlations due to the presence of the anharmonicity via a unitary operator which is determined by the variational principle.

I. INTRODUCTION

The great relevance that the study of anharmonic-oscillator models has in many branches of physics cannot be doubted. Interesting and important features of numerous systems are a consequence of the anharmonic nonlinear character of vibrations that occur in those systems. The corresponding literature is, consequently, quite abundant, and different aspects of the problem are the subject of much interesting work, both from the analytical and the numerical point of view. A small sample is that of Refs. 1–29.

The purpose of the present work is to develop a very simple approximate treatment of the D-dimensional, generalized anharmonic oscillator, defined by a Hamiltonian of the form

$$\hat{H}=\sum_{i=1}^{D}\left(-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x_i^{\,2}}+\frac{m}{2}\omega_i^{\,2}x_i^{\,2}\right)+\lambda V(x_1,x_2,\ldots,x_D)\,, \tag{1.1}$$

where V is an arbitrary *even* function of the coordinates, i.e.,

$$V(x_1,\ldots,x_k,\ldots,x_D)=V(x_1,\ldots,-x_k,\ldots,x_D) \tag{1.2}$$

for $1\leq k\leq D$ (subject to some restrictions stipulated in Sec. II).

The present work constitutes a generalization, to D dimensions, of a method recently proposed for the one-dimensional case.[30] The corresponding formalism is discussed in Sec. II. Moreover, a simple treatment of the anisotropic case is given in Sec. III. Different applications are presented in Sec. IV and conclusions are drawn in Sec. V.

II. FORMALISM

A. The mapping operator

We shall rewrite our Hamiltonian (in appropriate units) in the form

$$\hat{H}=-\nabla_D^{\,2}+\sum_{i=1}^{D}x_i^{\,2}+\lambda V(x_1,\ldots,x_D) \tag{2.1}$$

and postpone consideration of the anisotropic case to a later stage. An even more convenient expression can be given, by recourse to the definitions

$$\hat{H}_i^{(0)}=-\frac{\delta^2}{\delta x_i^{\,2}}+x_i^{\,2}\,,\quad i=1,\ldots,D\,, \tag{2.2}$$

$$\hat{H}^{(0)}=\sum_{i=1}^{D}\hat{H}_i^{(0)}\,, \tag{2.3}$$

and to the Taylor expansion of $V(x_1,\ldots,x_D)$

$$V(x_1,\ldots,x_D)=\sum_{j=0}^{\infty}\frac{1}{j!}\{\vec{r}\cdot\vec{\nabla}\}_{\vec{q}=0}^{(j)}V(q_1,\ldots,q_D)\,, \tag{2.4}$$

$\vec{r}$ being a vector whose components are $x_1,\ldots,x_D$ and $\vec{\nabla}$ one with components $\delta/\delta q_1,\ldots,\delta/\delta q_D$. In terms of the usual boson creation operators

$$\hat{a}_j^{\dagger}=\hat{p}_j+i\hat{x}_j\,,\quad j=1,\ldots,D\,, \tag{2.5}$$

and denoting by $\hat{B}_j$ the linear combination

$$\hat{B}_j=-i(\hat{a}_j^{\dagger}-\hat{a}_j)\,, \tag{2.6}$$

we can finally write $\hat{H}$ in the form ($\hat{1}$ is the unity operator)

$$\hat{H}=D\hat{1}+\sum_{i=1}^{D}\hat{a}_i^{\dagger}\hat{a}_i+\sum_{\vec{i}}\lambda_{\vec{i}}\prod_{j=1}^{D}\hat{B}_j^{i_j}\,, \tag{2.7}$$

where $\vec{i}$ stands for the set of integers $i_1,i_2,\ldots,i_D$, so that

$$\lambda_{\vec{i}}\equiv\frac{\lambda V^{(\vec{i})}(0)}{2^{i_1+\cdots+i_D}i_1!\,i_2!\cdots i_D!}\,, \tag{2.8}$$

$$V^{(\vec{i})}(0)=\frac{\delta^{\,i_1+i_2+\cdots+i_D}V}{\delta q_1^{\,i_1}\cdots\delta q_D^{\,i_D}}\bigg|_{\vec{q}=0}\,, \tag{2.9}$$

and

$$\sum_{\vec{i}}\equiv\sum_{i_1}\sum_{i_2}\cdots\sum_{i_D}\,. \tag{2.10}$$

It is possible thus to put $\hat{H}$ into the form

$$\hat{H}=\hat{H}^{(0)}+\sum_{\vec{i}}\lambda_{\vec{i}}\prod_{j=1}^{D}\hat{B}_j^{i_j}\,, \tag{2.11}$$

which suggests the idea of relating the eigenstates $|P'_1, P'_2, \ldots, P'_D\rangle$ of $\hat{H}$ to those $|r_1, r_2, \ldots, r_D\rangle$ of $\hat{H}_0$ by means of a mapping operator $\hat{F}_\infty(r_1, \ldots, r_D)$, as in Ref. 30,

$$|P'_1, P'_2, \ldots, P'_D\rangle = \exp[i\hat{F}_\infty(r_1, \ldots, r_D)]\,|r_1, \ldots, r_D\rangle \tag{2.12}$$

with (remembering that V is an *even* function)

$$\hat{F}_\infty(r_1, \ldots, r_D) = i\sum_{k=1}^{\infty}\sum_{n=1}^{D} h_n^{(k)}(r_1, \ldots, r_D) \times [(\hat{a}_n^\dagger)^{2k} - (\hat{a}_n)^{2k}]\,. \tag{2.13}$$

Minimization of

$$\langle P'_1 = 0, P'_2 = 0, \ldots, P'_D = 0\,|\,\hat{H}\,|\,P'_1 = 0, P'_2 = 0, \ldots, P'_D = 0\rangle \tag{2.14}$$

with respect to the quantities h of Eq. (2.13) would lead to the exact solution for the ground state (GS) of our system.[30]

Following Ref. 30 we shall propose an approximate procedure in which one retains the $k=1$ part of (2.13), thus working hereafter with a mapping operator defined by

$$\hat{F}(r_1, \ldots, r_D) = i\sum_{n=1}^{D} h_n(r_1, \ldots, r_D)[(\hat{a}_n^\dagger)^2 - (\hat{a}_n)^2] \equiv i\sum_{n=1}^{D} \hat{F}_n(r_1, \ldots, r_D)\,. \tag{2.15}$$

[In those occasions in which no confusion is likely to ensue we shall write simply $\hat{F}_j$ instead of $\hat{F}_j(r_1, \ldots, r_D)$ and h_j instead of $h_j(r_1, \ldots, r_D)$.]

This approximate mapping operator $\hat{F}$ will lead to approximations to the eigenstates of $\hat{H}$ given by

$$|P_1, P_2, \ldots, P_D\rangle = \exp[i\hat{F}(r_1, \ldots, r_D)]\,|r_1, \ldots, r_D\rangle\,, \tag{2.16}$$

which are to be obtained by minimization of

$$\epsilon_{r_1, \ldots, r_D} = \langle r_1, \ldots, r_D\,|\,\exp[-i\hat{F}(r_1, \ldots, r_D)]\,\hat{H}\exp[i\hat{F}(r_1, \ldots, r_D)]\,|\,r_1, \ldots, r_D\rangle \tag{2.17}$$

with respect to the quantities h of Eq. (2.15). This procedure will yield a rigorous upper bound to the GS energy

$$\epsilon_{0, \ldots, 0} = \langle P_1 = 0, P_2 = 0, \ldots, P_D = 0\,|\,\hat{H}\,|\,P_1 = 0, P_2 = 0, \ldots, P_D = 0\rangle\,. \tag{2.18}$$

B. Commutation rules

A simple algorithm can be devised which allows one to evaluate matrix elements of the type one finds on the right-hand side of (2.17).

Let us write

$$\hat{C}_0 \equiv \hat{H} \tag{2.19}$$

and define

$$\hat{C}_n = \{\hat{C}_{n-1}, \hat{F}\}\,. \tag{2.20}$$

If we also set

$$\hat{S}_0 \equiv \hat{H} - \hat{H}_0\,, \tag{2.21}$$

we see that $\hat{C}_n$ can be written in the form

$$\hat{C}_n = \sum_{k=1}^{D} \hat{C}_n^{(k)} + \hat{S}_n\,, \tag{2.22}$$

where

$$\hat{S}_n = \{\hat{S}_{n-1}, \hat{F}\}\,, \tag{2.23}$$

i.e., a part of $\hat{C}_n$ is separable, with a contribution $\hat{C}_n^{(k)}$ from each (dimensional) subindex k.

The usual commutation relationships

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = 2\delta_{ij}\,, \qquad \{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \tag{2.24}$$

lead to

$$\{\hat{H}_i^{(0)}, \hat{F}_j\} = 0\,, \quad 1 \le i \ne j \le D\,, \tag{2.25}$$

$$\{\hat{B}_i, \hat{F}_j\} = 0\,, \quad 1 \le i \ne j \le D\,, \tag{2.26}$$

$$\{\hat{B}_j^m, \hat{F}_j\} = -4imh_j\hat{B}_j^m\,, \quad 1 \le j \le D\,, \tag{2.27}$$

$$\{\hat{B}_i, \hat{B}_j\} = 0\,, \quad 1 \le i, j \le D\,, \tag{2.28}$$

$$\{\hat{H}_j^{(0)}, \hat{F}_j\} = 4ih_j[(\hat{a}_j^\dagger)^2 + (\hat{a}_j)^2]\,, \tag{2.29}$$

$$\{(\hat{a}_j^\dagger)^2 + (\hat{a}_j)^2, \hat{F}_j\} = 16ih_j(\hat{a}_j^\dagger\hat{a}_j + \hat{1})\,. \tag{2.30}$$

These commutation rules allow one to obtain a general expression for the $\hat{C}_n^{(k)}$:

$$\hat{C}_{2n}^{(k)} = (-1)^n 4^{3n} h_k^{2n}(\hat{a}_k^\dagger\hat{a}_k + \hat{1})\,, \tag{2.31}$$

$$\hat{C}_{2n+1}^{(k)} = i4^{3n+1}(-1)^n h_k^{2n+1}[(\hat{a}_k^\dagger)^2 + (\hat{a}_k)^2]\,. \tag{2.32}$$

The operator $\hat{S}_n$ can also be given a general form, starting with [cf. Eq. (2.11)]

$$\hat{S}_0 = \sum_{\vec{i}} \lambda_{\vec{i}} \prod_{j=1}^{D} \hat{B}_j^{i_j} \tag{2.33}$$

and employing (2.27). If we let $\vec{h}$ be a vector whose components are $h_1, h_2, \ldots, h_D$, and similarly we denote by $\vec{j}$ the vector of components $j_1, j_2, \ldots, j_D$, the following result ensues:

$$\left\{\prod_{j=1}^{D} \hat{B}_j^{i_j}, \hat{F}\right\} = -4i(\vec{j}\cdot\vec{h}) \prod_{k=1}^{D} \hat{B}_k^{j_k} \tag{2.34}$$

and, consequently,

$$\hat{S}_n = \sum_{\vec{j}} (-4i)^n \lambda_{\vec{j}} (\vec{j}\cdot\vec{h})^n \prod_{k=1}^{D} \hat{B}_k^{j_k} . \tag{2.35}$$

We are now in a position to give the commutators $\hat{C}_n$, after introducing

$$g_{\vec{j}}^n = \lambda_{\vec{j}} 4^n (\vec{j}\cdot\vec{h})^n , \tag{2.36}$$

the general expressions

$$\hat{C}_{2n} = (-1)^n 4^{3n} \sum_{k=1}^{D} h_k^{2n} (\hat{a}_k^\dagger \hat{a}_k + \hat{1}) + \sum_{\vec{j}} (-1)^n g_{\vec{j}}^{2n} \prod_{k=1}^{D} \hat{B}_k^{j_k} , \tag{2.37}$$

$$\hat{C}_{2n+1} = i\, 4^{3n+1} (-1)^n \sum_{k=1}^{D} h_k^{2n+1} [(\hat{a}_k^\dagger)^2 + (\hat{a}_k)^2] - i \sum_{\vec{j}} (-1)^n g_{\vec{j}}^{2n+1} \prod_{k=1}^{D} \hat{B}_k^{j_k} . \tag{2.38}$$

C. Matrix elements

The results of the previous subsection allow us to easily evaluate those matrix elements that are needed in order to obtain approximate values for the eigenvalues of $\hat{H}$. The following matrix elements are relevant for our purpose:

$$\langle r_1, \ldots, r_D | \hat{a}_j^\dagger \hat{a}_j | r_1, \ldots, r_D \rangle = 2 r_j , \quad j = 1, \ldots, D , \tag{2.39}$$

$$\langle r_1, \ldots, r_D | [(\hat{a}_j^\dagger)^2 + (\hat{a}_j)^2] | r_1, \ldots, r_D \rangle = 0 , \quad j = 1, \ldots, D , \tag{2.40}$$

$$\left\langle r_1, \ldots, r_D \middle| \prod_{j=1}^{D} \hat{B}_{jj}^{p_j} \middle| r_1, \ldots, r_D \right\rangle = \prod_{j=1}^{D} v_{r_j, p_j}^{j} , \quad 0 \le p_j \le \infty , \tag{2.41}$$

where

$$v_{r_j p_j}^{j} = \langle r_j | \hat{B}_{jj}^{p_j} | r_j \rangle = \frac{(2p_j)!}{(p_j)!} \sum_{k=0}^{r_j} 2^{r_j - k} \binom{p_j}{r_j - k} \binom{r_j}{k} \delta_{p_j \text{ even}} . \tag{2.42}$$

The approximate energy given by Eq. (2.17) can now be evaluated:

$$\epsilon_{r_1, \ldots, r_D}(\vec{h}) = \langle r_1, \ldots, r_D | e^{-i\hat{F}} \hat{H} e^{i\hat{F}} | r_1, \ldots, r_D \rangle = \sum_{n=0}^{\infty} \frac{i^n}{n!} \langle r_1, \ldots, r_D | \hat{C}_n | r_1, \ldots, r_D \rangle , \tag{2.43}$$

an expression that, according to Eqs. (2.36)–(2.42), leads to

$$\epsilon_{r_1, \ldots, r_D}(\vec{h}) = \sum_{k=1}^{D} (2 r_k + 1) \cosh(8 h_k) + \sum_{\vec{i}} V^{(2\vec{i})}(0) \prod_{j=1}^{D} \frac{\exp(8 i_j h_j)}{(i_j)!\, 2^{2 i_j}} \sum_{\alpha_j = 0}^{r_j} 2^{r_j - \alpha_j} \binom{i_j}{r_j - \alpha_j} \binom{r_j}{\alpha_j} , \tag{2.44}$$

which has the same structure as that of the corresponding one-dimensional case.[30]

Equation (2.44) can be simplified by recourse to the D-dimensional Laplace transform

$$f(\vec{h}) = f(h_1, \ldots, h_D) = \int_0^\infty \cdots \int_0^\infty \exp(-\vec{h}\cdot\vec{x}) f(\vec{x})\, dx_1 dx_2 \cdots dx_D . \tag{2.45}$$

It is then seen[30] that the Laplace transform f_V of $V(x_1^{1/2}, \ldots, x_D^{1/2})/(x_1 \cdots x_D)^{1/2}$ is given by

$$f_V(\vec{h}) = \pi^{D/2} \exp[4(h_1 + \cdots + h_D)] \times \sum_{\vec{i}} V^{(2\vec{i})}(0) \prod_{j=1}^{D} \frac{\exp(8 i_j h_j)}{2^{2 i_j} (i_j)!} , \tag{2.46}$$

which, after introducing the auxiliary function

$$\phi(\vec{h}) = \pi^{-D/2} \exp[4(h_1 + \cdots + h_D)] f_V(\vec{h}) , \tag{2.47}$$

allows us to write (2.44) in a specially compact form for the case $r_1 = \cdots = r_D = 0$,

$$\epsilon_{r_1 = 0, \ldots, r_D = 0} = \sum_{k=1}^{D} \cosh(8 h_k) + \lambda \phi(\vec{h}) . \tag{2.48}$$

As previously stated, this constitutes a (variational) upper bound to the ground-state energy, the variational parameters being the components of the vector $\vec{h}$.

For reasons of symmetry, we also obtain an upper bound in those cases in which just one of the r_i, for example, r_j, equals one, all the remaining r_i being equal to zero:

$$\epsilon_{r_1 = 0, \ldots, r_k = 1, \ldots, r_D = 0} = \sum_{j=1}^{D} (2\delta_{kj} + 1) \cosh(8 h_k) + \lambda \phi(\vec{h}) + \frac{\lambda}{4} \frac{\delta \phi}{\delta h_j} . \tag{2.49}$$

In general, of course, the method here proposed does not yield upper bounds to all the eigenvalues of $\hat{H}$. The second term of the right-hand side of Eq. (2.44) can be expressed in terms of $\phi(\vec{h})$ and its different partial derivatives with respect to the components of $\vec{h}$. As an example, we have

$$\epsilon_{1,\ldots,1}(\vec{h}) = 3\sum_{k=1}^{D}\cosh(8h_k) + \lambda\phi(\vec{h}) + \frac{\lambda}{4}\sum_{i=1}^{D}\frac{\delta\phi}{\delta h_i} + \frac{\lambda}{4^2}\sum_{i_1\neq i_2}\frac{\delta^2\phi}{\delta h_{i_1}\delta h_{i_2}} + \cdots + \frac{\lambda}{4^D}\sum_{i_1\neq\cdots\neq i_D}\frac{\delta^D\phi}{\delta h_{i_1}\cdots\delta h_{i_D}}. \quad (2.50)$$

We shall concern ourselves mainly with the approximate ground-state vector $|P_1=0,\ldots,P_D=0\rangle$.

III. THE ANISOTROPIC CASE

In order to apply the method developed in the previous section to the D dimensional anisotropic anharmonic oscillator, *we shall interpret any anisotropy as an anharmonic term.*

The original Hamiltonian is

$$\hat{H} = -\nabla_D{}^2 + \sum_{i=1}^{D}\omega_i{}^2 x_i{}^2 + \lambda V(x_1,\ldots,x_D) \quad (3.1)$$

and we shall select a given (nonzero) frequency, for example ω_1, and normalize with respect to it by introduction of the quantities

$$\alpha_i = \frac{\omega_i}{\omega_1}, \quad i=1,\ldots,D. \quad (3.2)$$

The Hamiltonian is now rewritten as

$$\hat{H} = -\nabla_D{}^2 + \sum_{i=1}^{D} x_i{}^2 + \lambda V(x_1,\ldots,x_D) + \sum_{i=1}^{D}(\alpha_i{}^2-1)x_i{}^2 = \hat{H}^{(0)} + W(x_1,\ldots,x_D) \quad (3.3)$$

with

$$W(x_1,\ldots,x_D) = \lambda V(x_1,\ldots,x_D) + \sum_{i=1}^{D}(\alpha_i{}^2-1)x_i{}^2. \quad (3.4)$$

On account of the linear character of the Laplace transform, the two contributions to W can be separately studied, i.e., we can write, in self-explanatory notation,

$$\phi_W = \phi_V + \phi_\alpha \quad (3.5)$$

with

$$\phi_\alpha(\vec{h}) = \tfrac{1}{2}\sum_{i=1}^{D}(\alpha_i{}^2-1)\exp(8h_i). \quad (3.6)$$

The approximate GS energy $\epsilon_{0,\ldots,0}\equiv\epsilon_0$ is thus obtained by minimization of

$$\epsilon_0(\vec{h}) = \sum_{k=1}^{D}[\cosh(8h_k) + \tfrac{1}{2}(\alpha_k{}^2-1)\exp(8h_k)] + \lambda\phi_V(\vec{h}) \quad (3.7)$$

with respect to the components h_k of the vector $\vec{h}$.

Equation (3.7) may be considered to constitute the main result of the present work since it presents us with a rigorous upper bound to the GS energy of an anisotropic D-dimensional anharmonic oscillator for any even anharmonicity V which admits of a Laplace transform.

IV. APPLICATIONS

A. The D-dimensional anisotropic harmonic oscillator

A well-known exact solution is available in this particular instance, which corresponds to the case in which $V(\vec{x})=0$ in Eq. (3.1).

Assuming $\omega_1\neq 0$ we can set $\omega_k=\alpha_k\omega_1$, for $2\leq k\leq D$. According to the results of Sec. III, the GS energy is obtained by minimization of

$$\epsilon_0(h_1,\ldots,h_D) = \sum_{k=1}^{D}\left[h_k(\tfrac{1}{2}+\beta_k{}^2) + \frac{1}{2h_k}\right] \quad (4.1)$$

with

$$\beta_k{}^2 = \tfrac{1}{2}(\alpha_k{}^2-1). \quad (4.2)$$

Thus, the "vector" $\vec{h}$ that minimizes (4.1) is the one whose components are given by

$$h_k = \frac{1}{\alpha_k}, \quad (4.3)$$

and our upper bound to the GS energy is then

$$\epsilon_0 = \sum_{k=1}^{D}\frac{\omega_k}{\omega_1}, \quad (4.4)$$

which *coincides with the exact result.*

B. Isotropic anharmonic case with $V(r)=r^{2N}$

Interesting studies concerning this problem can be found in Refs. 21 and 23. The anharmonicity is given by

$$V(x_1,\ldots,x_D) = \left(\sum_{i=1}^{D}x_i{}^2\right)^N, \quad (4.5)$$

whose associated function (cf. Sec. II) is

$$\phi(z_1,\ldots,z_D) = \frac{N!}{2^{2N}}\sum_{\vec{p}}\prod_{j=1}^{D}\binom{2p_j}{p_j}z^{p_j}, \quad (4.6)$$

where, as before,

$$\sum_{\vec{p}} \equiv \sum_{p_1=0}^{N}\cdots\sum_{p_D=0}^{N}, \quad (4.7)$$

and the restriction

$$\sum_{j=1}^{D}p_j = N \quad (4.8)$$

is to be obeyed. As all z_i are essentially equiva-

lent, it is not too unreasonable to set $z_1=z_2=\cdots=z_D=z$, and thus obtain our approximate GS energy ϵ_0 by minimizing with respect to z the expression

$$\epsilon_0(z)=\frac{D}{2}\left(z+\frac{1}{z}\right)+\lambda a_{N,D}z^N \tag{4.9}$$

with

$$a_{N,D}=\frac{N!}{2^{2N}}\sum_{\vec{p}}\prod_{j=1}^{D}\binom{2p_j}{p_j}. \tag{4.10}$$

Notice that an *analytical* solution obtains for $N=0$, 1, 2, 3, and 5. Of particular interest on account of its applications is the case $N=2$ (see Refs. 24 and 25). Notice that in this instance the following particularly simple expressions hold:

$$a_{2,D}=\frac{D}{4}(D+2), \tag{4.11}$$

$$\epsilon_0(N=2,z)=\frac{D}{2}\left(z+\frac{1}{z}\right)+\frac{D}{4}\lambda(D+2)z^2. \tag{4.12}$$

Table I exhibits the corresponding results for $D=3$, which are compared to the ones obtained by Ehlenberg and Mendelsohn[21] employing Padé approximants. The agreement between both sets of results is excellent.

C. A special anisotropic case

We shall consider now the following anharmonicity

$$V(\vec{r})=\sum_{i=1}^{D}\sum_{j=1}^{D}a_{ij}x_i^2x_j^2, \tag{4.13}$$

which, for $D=2$, has been extensively studied by Hioe *et al.*[26] The associated ϕ function is

$$\phi(z_1,\ldots,z_D)=\tfrac{1}{4}\sum_{i=1}^{D}\sum_{j=1}^{D}(2\delta_{ij}+1)a_{ij}z_iz_j, \tag{4.14}$$

which leads to

$$\epsilon_0(z_1,\ldots,z_D)=\tfrac{1}{2}\sum_{i=1}^{D}\left[z_i+\frac{1}{z_i}+\frac{\lambda}{2}\sum_{j=1}^{D}(2\delta_{ij}+1)a_{ij}z_iz_j\right], \tag{4.15}$$

which is to be minimized with respect to the z_i. We shall compare to those of Hioe *et al.* (for $D=2$) our results for the GS and for the first two excited states, i.e., ϵ_{00}, ϵ_{01}, and ϵ_{11}. This is done in Tables II–VI. The agreement between our approximate results and the exact ones of Hioe *et al.* is very good.

In the special case of "spherical coupling" (Hioe *et al.*, Ref. 26)

$$a_{11}=a_{22}=\cdots=a_{DD}=a, \qquad a_{ij}=b \text{ for all } i\neq j, \tag{4.16}$$

one can guess *a priori* that, on account of the symmetry introduced by (4.16), the values of z_i which minimize the GS energy will be characterized by the property

$$z_1=z_2=\cdots=z_D=z. \tag{4.17}$$

Our problem then reduces itself to the one-dimensional one. The corresponding task is thus that of minimizing

$$\epsilon_0(z)=D\left[\frac{1}{2}\left(z+\frac{1}{z}\right)+\frac{\lambda}{4}[b(D-1)+3a]z^2\right] \tag{4.18}$$

with respect to z. This expression coincides with the corresponding one of Sec. IV B for $a=b=1$.

TABLE I. Results for the three-dimensional anharmonic (isotropic) oscillator, where the anharmonicity is of the form λr^{2N}. For different values of the anharmonic coupling constant λ, the second column displays the GS energies obtained with the present approach, which are compared to those of Ehlenberger and Mendelsohn (third column). The agreement (%) between the two sets of results is exhibited in the last column.

λ	E_{BEP}	E_{EM}	%
0.01	1.518303	1.518263	99.99
0.05	1.584259	1.583613	99.95
0.2	1.773386	1.769503	99.78
1	2.339118	2.322655	99.29

TABLE II. Ground-state energies for the anharmonic, anisotropic case ($D=2$) of Eq. (4.3), for different anisotropies [as given by the parameter a_{12} (see text)], as functions of the corresponding coupling constant λ. In all cases the upper figure is obtained with the techniques described in the text, while the bottom one has been taken from the work of Hioe *et al.*[26] The degree of agreement (%) between the two treatments is displayed to the right of these numbers. $a_{11}=a_{22}=1$.

λ \ a_{12}	1		0		−1	
0.05	1.0853 1.0843	99.91	1.0662 1.0653	99.91	1.0457 1.0443	99.86
0.1	1.1526 1.1502	99.79	1.1206 1.1183	99.79	1.0853 1.0813	99.63
0.5	1.4864 1.4760	99.30	1.4033 1.3924	99.22	1.3053 1.2808	98.12
1	1.7401 1.7242	99.08	1.6250 1.6075	98.92	1.4864 1.4438	97.13
10	3.3466 3.3012	98.64	3.0625 3.0100	98.28	2.7091 2.5577	94.41
100	7.0161 6.9119	98.51	6.3848 6.2628	98.08	5.5937 5.2248	93.40

TABLE III. Energies of the first excited state, in the anharmonic, anisotropic case described by Eq. (4.3). All remaining details are similar to those described in the caption of Table II.

λ \ a_{12}	1		0		−1	
0.05	2.2412 2.2388	99.89	2.1890 2.1861	99.86	2.1324 2.1248	99.64
0.1	2.4196 2.4143	99.78	2.3355 2.3286	99.70	2.2412 2.2120	98.69
0.5	3.2500 3.2315	99.43	3.0479 3.0206	99.10	2.8066 2.6984	96.14
1	3.8576 3.8304	99.29	3.5832 3.5417	98.83	3.2500 3.0666	94.35
5	6.1250 6.0692	99.08	5.6128 5.5242	98.42	4.9772 4.5136	90.68
100	16.034 15.869	98.97	14.585 14.319	98.17	12.769 11.217	87.84

TABLE IV. Energy of the excited state ϵ_{11} in the anharmonic, anisotropic case described by Eq. (4.3). All remaining details are similar to those described in the caption of Table II.

λ \ a_{12}	1		0		−1	
0.05	3.4580 3.4542	99.88	3.3103 3.3069	99.89	3.1373 3.1289	99.73
0.1	3.7802 3.7723	99.79	3.5467 3.5390	99.78	3.2560 3.2327	99.28
0.5	5.2204 5.1953	99.52	4.6782 4.6488	99.37	3.9160 3.7746	96.38
1	6.2498 6.2140	99.42	5.5198 5.4759	99.20	4.4592 4.2106	94.42
5	10.039 9.9687	99.28	8.6913 8.5991	98.93	6.6479 5.9848	90.02
100	26.444 26.237	99.21	22.649 22.375		16.781 14.489	86.34

The minimization problem posed by Eq. (4.18) can, of course, be solved analytically, providing us with simple expressions for *any* values of D and λ no matter how large they may be.

In particular, if we call $e_0=\epsilon_0/D$ we obtain the following results in the limit of very large λ:

$$e_0(a=1,b=0)\underset{\lambda\gg1}{\longrightarrow}\frac{3^{4/3}}{4}\lambda^{1/3} \tag{4.19}$$

and

$$e_0(a=1,b=1)\underset{D\gg1}{\overset{\lambda\gg1}{\longrightarrow}}\tfrac{3}{4}(\lambda D)^{1/3} \tag{4.20}$$

so that the ratio between the coupled spherical result ($a=1,b=1$) and the uncoupled one ($a=1$, $b=0$) becomes independent of the coupling constant λ:

$$c=\frac{e_0(a=1,b=1)}{e_0(a=1,b=0)}\underset{D\gg1}{\overset{\lambda\to\infty}{\longrightarrow}}\frac{D^{1/3}}{3^{1/3}}\simeq0.693D^{1/3}. \tag{4.21}$$

This result is to be compared to that estimated by Hioe *et al.*, $c=0.738D^{1/3}$. Hioe *et al.* have rigorously shown, for the case $D=2$, that both $e_0(a=1,b=1)$ and $e_0(a=1,b=0)$ grow as $\lambda^{1/3}$ for λ large enough.[28] Our *approximate* results (4.19) and (4.20) display the same behavior, but for *any* D.

We show in Table VII results for $e_0(a=1,b=1)$, i.e., for the ground-state energy of D coupled oscillators ($\lambda=1$), both in order to illustrate the corresponding energetic behavior and the power of our approach.

It is easy to extend our treatment to the following generalization of the anharmonicity (4.13)

$$V(x_1,\ldots,x_D)=\sum_{n=0}^{N}\sum_{m=0}^{M}\sum_{i=1}^{D}\sum_{j=1}^{D}a_{ij}^{(n,m)}x_i^{2n}x_j^{2m}, \tag{4.22}$$

the associated ϕ function being

$$\phi(z_1,\ldots,z_D)=\sum_{n=0}^{N}\sum_{m=0}^{M}\frac{1}{4^{n+m}}\left(\sum_{i=1}^{D}a_{i,i}^{(n,m)}\frac{[2(n+m)]!}{(n+m)!}z_i^{n+m}+\sum_{i\neq j}^{D}a_{ij}^{(n,m)}\frac{(2n)!(2m)!}{n!m!}z_i^{n}z_j^{m}\right). \tag{4.23}$$

D. The doubly anharmonic oscillator

As a final example we shall discuss the following anharmonicity which has been studied in the one-dimensional case[16-20] but not, as far as we know, in the D-dimensional one,

$$V(r)=\lambda_1r^4+\lambda_2r^6,\qquad r^2=\sum_{i=1}^{D}x_i^2. \tag{4.24}$$

Here we also have "spherical" symmetry and, consequently, just one variational parameter z,

$$\phi(z)=\lambda_1a_{2,D}z^2+\lambda_2a_{3,D}z^3 \tag{4.25}$$

with

$$a_{2,D}=\tfrac{1}{2}D(D+2),\qquad a_{3,D}=\tfrac{1}{8}D(D+2)(D+4). \tag{4.26}$$

The GS energy arises from the minimization of

$$\epsilon_0=\frac{D}{2}\left(z+\frac{1}{z}\right)+\frac{\lambda_1}{2}D(D+2)z+\frac{\lambda_2}{8}D(D+2)(D+4)z^3. \tag{4.27}$$

TABLE V. Ground-state energies for the anharmonic, anisotropic case of Eq. (4.3) for $a_{11}=0.8$, $a_{22}=1$. All remaining details are similar to those of Table II.

λ \ a_{12}	1		0.8		0.6		0.4		0.2		0	
0.05	1.0787 1.0796	99.92	1.0750 1.0758	99.92	1.0712 1.0720	99.93	1.0673 1.0681	99.93	1.0634 1.0641	99.93	1.0594 1.0601	99.93
0.1	1.1409 1.1432	99.80	1.1347 1.1368	99.82	1.1284 1.1303	99.83	1.1218 1.1238	99.82	1.1151 1.1170	99.83	1.1082 1.1102	99.82
0.3	1.3215 1.3281	99.50	1.3092 1.3156	99.51	1.2966 1.3027	99.53	1.2834 1.2895	99.53	1.2697 1.2759	99.51	1.2553 1.2619	99.48
0.5	1.4523 1.4621	99.33	1.4363 1.4457	99.35	1.4196 1.4288	99.36	1.4023 1.4115	99.35	1.3841 1.3935	99.33	1.3649 1.3750	99.27
0.7	1.5587 1.5709	99.22	1.5398 1.5517	99.23	1.5202 1.5318	99.24	1.4997 1.5113	99.23	1.4781 1.4901	99.19	1.4553 1.4681	99.13
1	1.6913 1.7065	99.11	1.6691 1.6839	99.12	1.6460 1.6605	99.13	1.6217 1.6363	99.11	1.5961 1.6112	99.06	1.5689 1.5852	98.97
5	2.6117 2.6450	98.74	2.5692 2.6017	98.75	2.5245 2.5568	98.73	2.4773 2.5102	98.69	2.4272 2.4616	98.60	2.3734 2.4109	98.44
10	3.2200 3.2641	98.65	3.1652 3.2083	98.65	3.1075 3.1505	98.64	3.0465 3.0903	98.58	2.9815 3.0275	08.48	2.9118 2.9620	98.30
50	5.3693 5.4490	98.54	5.2730 5.3512	98.54	5.1716 5.2496	98.51	5.0642 5.1439	98.45	4.9495 5.0335	98.33	4.8260 4.9180	98.13
100	6.7314 6.8330	98.51	6.6095 6.7092	98.51	6.4811 6.5805	98.49	6.3449 6.4465	98.42	6.1996 6.3067	98.30	6.0429 6.1604	98.09
500	11.446 11.622	98.48	11.237 11.409	98.49	11.016 11.188	98.46	10.781 10.958	98.39	10.531 10.717	98.26	10.261 10.465	98.05
5000	24.604 24.984	98.48	24.151 24.524	98.48	23.674 24.047	98.45	23.168 23.549	98.38	22.627 23.030	98.25	22.044 22.486	98.03

TABLE VI. Ground-state energies for the case $a_{11}=0.4$, $a_{22}=1$. For further details see Table II.

λ \ a_{12}	0.8		0.6		0.4		0.2		0	
0.05	1.0630 1.0637	99.94	1.0590 1.0597	99.94	1.0550 1.0556	99.94	1.0509 1.0515	99.95	1.0467 1.0473	99.94
0.1	1.1141 1.1158	99.85	1.1073 1.1089	99.85	1.1004 1.1019	99.87	1.0933 1.0947	99.87	1.0859 1.0874	99.86
0.3	1.2662 1.2717	99.57	1.2524 1.2574	99.60	1.2379 1.2427	99.61	1.2227 1.2275	99.61	1.2066 1.2117	99.58
0.5	1.3788 1.3870	99.41	1.3604 1.3681	99.44	1.3410 1.3484	99.45	1.3204 1.3279	99.43	1.2986 1.3066	99.39
0.7	1.4713 1.4817	99.30	1.4494 1.4592	99.33	1.4262 1.4357	99.34	1.4016 1.4112	99.32	1.3752 1.3856	99.25
1	1.5875 1.6006	99.18	1.5614 1.5738	99.21	1.5338 1.5459	99.22	1.5043 1.5166	99.19	1.4725 1.4859	99.10
5	2.4072 2.4370	98.78	2.3558 2.3844	98.80	2.3008 2.3290	98.79	2.2413 2.2706	98.71	2.1762 2.2087	98.52
10	2.9548 2.9946	98.67	2.8881 2.9264	98.69	2.8165 2.8545	98.67	2.7390 2.7786	98.57	2.6538 2.6979	98.36
50	4.9005 4.9732	98.54	4.7825 4.8527	98.55	4.6556 4.7256	98.52	4.5177 4.5910	98.40	4.3654 4.4475	98.15
100	6.1369 6.2297	98.51	5.9873 6.0769	98.53	5.8263 5.9158	98.49	5.6512 5.7449	98.37	5.4577 5.5629	98.11
500	10.422 10.583	98.48	10.165 10.320	98.50	9.8871 10.042	98.45	9.5851 9.7481	98.33	9.2509 9.4342	98.06
5000	22.391 22.740	98.47	21.834 22.171	98.48	21.234 21.571	98.44	20.581 20.935	98.31	19.859 20.256	98.04

TABLE VII. Ground-state energy of D coupled oscillators (in units of D) for $\lambda=1$ [see Eq. (4.18)].

D	e_0/D
1	1.4033
2	1.4864
3	1.5594
4	1.6250
5	1.6849
10	1.9288
100	3.6105
1000	7.5549
10^5	34.823
10^{20}	3 481 192
10^{40}	1.6158×10^{13}
10^{50}	3.4812×10^{16}
10^{90}	7.5×10^{29}

V. CONCLUSIONS

A simple variational procedure has been presented which allows one to obtain an *approximation* to the energies and wave functions of the Hamiltonian (1.1). The method is based upon the idea of introducing into the uncorrelated harmonic-oscillator states the correlations induced by the presence of anharmonic terms via a unitary operator $e^{i\hat{F}}$, which is determined by the variational principle. This approach can be applied to any *even* function of the D coordinates that admits of a Laplace transform. In particular, it is seen that our treatment is able to deal with anisotropies by considering them as special types of anharmonicities. A rigorous upper bound to the GS of the Hamiltonian (1.1) is provided by the present approximation.

Some advantages of the present approach deserve special comment. It allows one to deal, in a very simple way, with the whole unperturbed basis, without truncating it. The numerical work involved is, in most instances, quite simple. Neither difficult numerical integrations nor large diagonalizations (as required by other methods) are necessary here (as a matter of fact, all calculations reported here where carried out with a Texas Instruments TI59 calculator). Furthermore, in many interesting cases the solution can be found *analytically* and, consequently, large values of λ or D do not pose any problem. Finally, comparison with exact results, as illustrated in Sec. IV, shows that our approximation yields rather good results. One may thus assert that our method may prove to be useful to obtain upper bounds to the GS energy in those cases in which exact treatments become too involved and, in other situations, provides a quick estimate of the corresponding results.

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