PHYSICAL REVIEW D VOLUME 33, NUMBER 6 15 MARCH 1986

Temperature-dependent anharmonic oscillator: A Hartree approach

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(Received 25 June 1985)

A temperature-dependent Hartree approach is studied with reference to the anharmonic-oscillator problem and shown to provide a good upper bound to the exact free energy. Alternative upper bounds are proposed and discussed.

I. INTRODUCTION

The generalized anharmonic oscillator poses a problem of permanent interest for a variety of reasons, as, for example, the prevailing belief that it may lead to a fuller understanding of "equivalent" models in field theory. A vast literature is available, a small sample being some works published recently.[1-5] The concomitant problem that is posed when such a system is heated has received less attention, although it certainly merits some consideration.[6-8] Within this spirit, in the present effort we wish to generalize to a finite temperature T a Hartree approximation for bosons recently proposed in Ref. 5.

The paper is organized as follows. The formalism is developed in Sec. II, while specific applications that illustrate it are presented in Sec. III. Alternative upper bounds to the exact free energies are discussed in Sec. IV and some conclusions are drawn in Sec. V.

II. THE FINITE-TEMPERATURE HARTREE APPROACH

Let us consider the Hamiltonian

$$\begin{aligned}\hat{H}&=\tfrac{1}{2}(\hat{P}^2+\hat{Q}^2)+V(\hat{Q})\\&=a^\dagger a+\tfrac{1}{2}+V\left[\frac{a^\dagger+a}{2}\right],\end{aligned} \tag{1}$$

where $V(\hat{Q})$, the potential, is assumed to admit a series expansion, while $a^\dagger$ and a are the usual boson creation and annihilation operators:

$$\begin{aligned}&a^\dagger=(\hat{Q}-i\hat{P})/\sqrt{2},\quad a=(\hat{Q}+i\hat{P})/\sqrt{2}\,,\\&\hat{Q}=(a^\dagger+a)/\sqrt{2},\quad \hat{P}=(a-a^\dagger)/\sqrt{2}i\,.\end{aligned} \tag{2}$$

If we set both $\hbar$ and the Boltzmann constant equal to unity, we can express the *exact* free energy F of our system in terms of the (normalized) density operator $\hat{\rho}_{\text{trial}}$ as[9]

$$F=\langle\hat{F}\rangle=\langle\hat{H}-T\hat{S}\rangle=\underset{\hat{\rho}_{\text{trial}}}{\text{Min}}\,\text{Tr}(\hat{\rho}_{\text{trial}}\hat{F})\,, \tag{3}$$

where $S=-\ln\hat{\rho}_{\text{trial}}$ is the so-called entropy operator. We know from statistical mechanics that $\hat{\rho}_{\text{exact}}$ is proportional to $\exp(-\hat{H}/T)$ and that F is of the form

$$F=-T\ln\text{Tr}[\exp(-\hat{H}/T)]\,. \tag{3$'$}$$

We wish here to develop a finite-temperature Hartree approximation for F, on the basis of the ideas put forward by Hsue and Chern,[5] appropriately generalized so as to allow for thermal effects.

The central idea that underlies the Hartree scheme is that of working with a one-body density matrix $\hat{\rho}$. Consequently, the temperature-dependent Hartree approximation (TDHA) for F will entail performing the minimization of Eq. (3) within the set of one-body density operators:

$$\hat{\rho}\propto\exp(-wb^\dagger b/T)\,, \tag{4}$$

where $b^\dagger$ and b are boson operators related to the "old" ones $(a^\dagger,a)$ by means of a Bogoliubov transformation:

$$\begin{aligned}&b^\dagger=\cosh(z)a^\dagger-\sinh(z)a\,,\\&b=\cosh(z)a-\sinh(z)a^\dagger\,.\end{aligned} \tag{5}$$

Both z and the frequency w are determined by the variational principle and are temperature dependent $[z=z(T),\ w=w(T)]$. The transformation (5) is, obviously, a scaling one, as it reads

$$\hat{Q}'=\exp(-z)\hat{Q},\quad \hat{P}'=\exp(z)\hat{P}\,, \tag{5$'$}$$

in terms of the "new" coordinates $\hat{Q}'$ and $\hat{P}'$ that can be constructed, after the fashion (2), out of $b^\dagger$ and b. Neither (5) nor (5$'$) provide us with the most general transformation: for instance, a constant term might be added to $b^\dagger$ and b in (5), which would account for a *translation* of the coordinate system. This type of transformation will be of no help here, as we shall deal only with symmetric, even potentials $V(\hat{Q})$:

$$V(\hat{Q})=\sum_{m=0}^{\infty}V^{(2n)}(0)\hat{Q}^{2n}/(2n)!\,. \tag{1$'$}$$

A straightforward application of Wick's theorem allows us now to evaluate $\langle\hat{H}\rangle\equiv\text{Tr}(\hat{\rho}\hat{H})$ by recourse to the finite-temperature single-particle (SP) density matrix:

$$\begin{aligned}\langle b^\dagger b\rangle&=\text{Tr}(\hat{\rho}b^\dagger b)\\&=[\exp(w/T)-1]^{-1}\\&\equiv f,\\\langle b^{\dagger 2}\rangle&=\langle b^2\rangle=0\,,\end{aligned} \tag{6}$$

where f is the *Bose occupation number*. Equation (6) allows us to easily obtain all quantities of interest for our present purposes, as, for instance,

$$\langle \hat{Q}^2\rangle=\tfrac{1}{2}[\cosh(z)+\sinh(z)]^2\langle(b^\dagger+b)^2\rangle$$
$$=2h(f+\tfrac{1}{2})\ , \tag{7a}$$

with

$$h=\tfrac{1}{2}[\cosh(z)+\sinh(z)]^2=\tfrac{1}{2}\exp(+2z)\ , \tag{7b}$$

and, more generally, by employing a well-known theorem about normal ordering[5,10]

$$(b^\dagger+b)^n=\sum_{j=0}^{[n/2]}:(b^\dagger+b)^{n-2j}:\frac{n!}{(n-2j)!2^j j!} \tag{8}$$

(with n a positive integer), one finds

$$\langle \hat{Q}^{2n}\rangle=h^n\langle(b^\dagger+b)^{2n}\rangle$$
$$=h^n(f+\tfrac{1}{2})^n\frac{(2n)!}{n!}\ . \tag{9}$$

In the last line of (9) we have used the result

$$\langle :(b^\dagger+b)^{2n}:\rangle=\frac{(2n)!}{n!}f^n\ , \tag{9'}$$

which Wick's theorem gives in a straightforward fashion. It is also obvious that

$$\langle \hat{Q}^{2n+1}\rangle=0\ ,$$
$$\langle \hat{Q}^{2n}\rangle=\langle \hat{Q}^2\rangle^n\frac{(2n)!}{2^n n!}\ , \tag{9''}$$

which implies that one might apply Wick's theorem to the Hermitian operator $\hat{Q}$, as $[(2n)!/n!2^n]$ is just the number of possible (n) contractions $\langle \hat{Q}^2\rangle$ out of $2n\hat{Q}$'s.

Analogously, we have

$$\langle \hat{P}^2\rangle=(f+\tfrac{1}{2})/2h\ , \tag{10}$$

$$\langle \hat{P}^{2n}\rangle=(4h)^{-n}(f+\tfrac{1}{2})^n\frac{(2n)!}{n!}$$
$$=\frac{(2n)!}{n!2^n}\langle \hat{P}^2\rangle^n\ , \tag{11}$$

$$\langle \hat{P}^{2n+1}\rangle=0\ , \tag{12}$$

and, using now the results (9),

$$\langle V(\hat{Q})\rangle=\sum_{n=0}^{\infty}\frac{V^{(2n)}(0)}{(2n)!}\langle \hat{Q}^{2n}\rangle$$
$$=\sum_{n=0}^{\infty}V^{(2n)}(0)(f+\tfrac{1}{2})^n(h^n/n!)$$
$$=\frac{2}{\sqrt{4\pi t}}\int_0^\infty \exp(-x^2/4t)V(x)dx$$
$$=\frac{1}{\sqrt{4\pi t}}\int_0^\infty \exp(-s/4t)\frac{V(\sqrt{s})}{\sqrt{s}}ds\ , \tag{13}$$

where the abbreviation $t=h(f+\frac{1}{2})$ has been utilized, together with the result

$$\frac{2}{\sqrt{4\pi t}}\int_0^\infty \exp(-x^2/4t)x^{2n}dx=\frac{t^n}{n!}(2n)!\ . \tag{13'}$$

As the entropy attains the well-known SP result

$$S=-\operatorname{Tr}\hat{\rho}\ln\hat{\rho}$$
$$=-[f\ln(f)-(f+1)\ln(f+1)]\ , \tag{14}$$

we are now in a position to evaluate $F=\langle \hat{F}\rangle$ and perform the corresponding minimization with respect to both h and f (or, equivalently, z and w). Noticing that $\langle V(\hat{Q})\rangle$ depends only upon t we obtain the set of equations

$$0=\frac{\partial' F}{\partial h}=(f+\tfrac{1}{2})\left[\frac{d}{dt}\langle V(Q)\rangle+1-1/4h^2\right]\ , \tag{15a}$$

$$0=\frac{\partial F}{\partial f}=T\ln[f/(1+f)]+1/2h\ , \tag{15b}$$

and, after solving for f in (15b), we find for w

$$w=1/2h\ , \tag{16}$$

which implies

$$f=1/[\exp(1/2hT)-1]\ , \tag{16'}$$

so that one is led to the following equation for h:

$$\frac{-1}{4h^2}+1+\frac{d}{dt}\langle V(\hat{Q})\rangle=0\ . \tag{17}$$

The method presented here provides us with an *upper bound* to the *exact* free energy, since we are minimizing (3) with respect to a restricted set of density operators.

It is worth noticing that, at $T=0$, f vanishes, so that (13) and (17) yield expressions already obtained for the ground state of an anharmonic oscillator by Bozzolo and Plastino.[11]

Our present expressions for finite-temperature expectation values [cf. Eqs. (11) and (13), for instance] attain identical aspect as the corresponding ones for $T=0$ (Ref. 11). More specifically, (13) yields the mean value of $V(\hat{Q})$ for Gaussian wave functions (ground state of the harmonic oscillator), but with a temperature-dependent width (or standard deviation), which is a consequence of the scaling operation (5′). One could thus speak, within the TDHA framework, of "effective," or "temperature-dependent" wave functions, that are able to mimic some of the features of statistical ensembles.

III. APPLICATION

As a specific example, let us consider the particular case $V(\hat{Q})=\lambda\hat{Q}^{2n}$. By application of the recipes (7)–(17) one is led to

$$F=(f+\tfrac{1}{2})(1/4h+h)+\lambda' h^n(f+\tfrac{1}{2})^n$$
$$+T[f\ln(f)-(f+1)\ln(f+1)]\ , \tag{18}$$

where h must satisfy

$$-1/4h^2+1+n\lambda'[h(f+\tfrac{1}{2})]^{(n-1)}=0\ , \tag{17'}$$

with $\lambda'=\lambda(2n)!/n!$ and f defined in expression (16′).

These expressions may be simplified for $T\to 0$ and $T\to\infty$. In the first case, we see from (16′) that f approaches 0 as $\exp(-1/2hT)$. Replacing for h the $T=0$

value we can easily obtain the limiting expressions for various thermodynamics quantities. For instance, the specific heat $C_v = T\partial S/\partial T$ vanishes as $\exp(-1/2hT)/(2hT)^2$, which is indeed the appropriate behavior.[7]

On the other hand, for $T \rightarrow \infty$, $f \rightarrow \infty$ while $h \rightarrow 0$. From Eq. (17′) we attain the asymptotic expressions

$$h = cT^{(1-n)/2n}, \quad f = 2hT = 2cT^{(n+1)/2n} , \tag{19}$$

with $c = 1/[2(2\lambda_n')^{1/n}]^{1/2}$. Utilizing (19) it is easy to obtain

$$\begin{gathered} \left\langle \frac{\hat{P}^2}{2} \right\rangle = T/2, \quad \left\langle \frac{\hat{Q}^2}{2} \right\rangle = 2c^2 T^{1/n} , \\ \langle \hat{Q}^{2n} \rangle = T/2n , \\ S = 1 + \ln 2c + \frac{(n+1)}{2n} \ln(T), \quad C_v = \frac{n+1}{2n} . \end{gathered} \tag{20}$$

It is important to realize that the leading terms of these limiting high-temperature expressions *coincide* with exact results (which may be obtained using the classical partition function, as in Ref. 8). The TDHA approach is exact in the classical limit. It is worthwhile mentioning that formulas (20) are valid for any $V(\hat{Q})$ which is a polynomial of degree $2n$ as the high-temperature behavior is dominated by the highest term ($\lambda \hat{Q}^{2n}, \lambda \geq 0$).

IV. ALTERNATIVE UPPER BOUNDS

Some additional upper bounds to F_{exact} will now be introduced, so as to place the TDHA in a clearer perspective. We start with the inequality[12]

$$\langle n \mid \exp(-\hat{H}/T) \mid n \rangle \geq \exp[-(\langle n \mid \hat{H} \mid n \rangle)/T] , \tag{21}$$

where $| n \rangle$ stands for any normalized state. A simple upper bound is thus immediately obtained by setting

$$| n \rangle = \frac{b^{\dagger n} | 0 \rangle}{\sqrt{n!}} \tag{22}$$

so that

$$F_{\text{exact}} \leq -T \ln \left[\sum_{n=0}^{\infty} \exp[-(\langle n \mid \hat{H} \mid n \rangle)/T) \right] . \tag{23}$$

If we choose $| 0 \rangle$ and $b^\dagger$ as, respectively, the vacuum and SP creation operator of the $T=0$ Hartree approach,[5] requiring, that h verifies the $T=0$ extremum condition (17), one finds

$$\begin{gathered} -1/4h^2 + 1 + \frac{d}{dt} \langle V(Q) \rangle = 0 , \\ t = \tfrac{1}{2} h = 1/4w . \end{gathered} \tag{24}$$

For $V(\hat{Q}) = \lambda \hat{Q}^4$ one is led to

$$F \leq -T \ln \left[\sum_{n=0}^{\infty} \exp\{-[1/4h + h + 6\lambda h^2 + 2n(h + 1/4h + 12\lambda h^2) + 12\lambda h^2 n(n-1)]/2T\} \right] . \tag{25}$$

TABLE I. Free energies (F), mean energies (E), and specific heats (C_v) obtained for different theoretical treatments in the case λQ^4 ($\lambda = 1.0$).

T	Treatment	F	E	C_v
0.5	TDHA	0.803 438 45	0.848 546 23	0.286 625 94
	Bound 1	0.803 388 25	0.848 819 45	0.289 133 42
	Bound 2	0.803 322 45	0.849 272 88	0.291 274 81
	Ref. 7	0.792 445 59	0.843 111 95	0.311 893 55
	Exact	0.793 352 95	0.844 036 66	0.311 726 43
1.0	TDHA	0.677 889 76	1.089 759 1	0.605 957 57
	Bound 1	0.677 748 86	1.086 887 6	0.584 458 57
	Bound 2	0.674 274 48	1.098 814 8	0.598 457 37
	Ref. 7	0.656 060 08	1.097 675 8	0.629 009 01
	Exact	0.657 104 88	1.098 003 4	0.627 050 64
2.5	TDHA	−0.470 869 06	2.136 646 0	0.735 841 56
	Bound 1	−0.429 614 68	2.039 079 6	0.642 934 20
	Bound 2	−0.499 209 94	2.187 828 9	0.695 321 42
	Ref. 7	−0.549 716 11	2.162 227 5	0.741 275 61
	Exact	−0.546 264 65	2.160 695 9	0.741 049 67
6.5	TDHA	−6.294 233 6	5.140 877 6	0.756 423 09
	Bound 1	−5.773 637 5	4.527 177 4	0.604 886 74
	Bound 2	−6.398 734 8	5.220 946 5	0.701 276 88
	Ref. 7	−6.547 166 9	5.175 821 1	0.757 709 74
	Exact	−6.536 521 3	5.176 460 7	0.758 438 93

TABLE II. Free energies (F), mean energies (E), and specific heats (C_v) obtained for different theoretical treatments in the case λQ^6 ($\lambda = 1.0$).

T	Treatment	F	E	C_v
0.5	TDHA	0.832 803 99	0.860 477 37	0.204 784 61
	Bound 1	0.832 750 96	0.860 858 95	0.209 897 86
	Bound 2	0.832 667 67	0.861 511 28	0.213 594 29
	Exact	0.797 038 80	0.837 659 64	0.269 146 24
1.0	TDHA	0.741 849 63	1.056 715 1	0.515 723 82
	Bound 1	0.740 414 02	1.056 771 4	0.493 277 33
	Bound 2	0.733 905 58	1.079 590 2	0.515 311 24
	Exact	0.679 753 29	1.067 520 3	0.572 970 08
2.5	TDHA	−0.190 242 49	1.968 271 2	0.645 010 09
	Bound 1	−0.140 892 92	1.826 921 2	0.499 283 27
	Bound 2	−0.264 157 73	2.069 364 6	0.582 483 05
	Exact	−0.393 156 89	2.025 144 4	0.660 825 98
6.5	TDHA	−5.094 053 9	4.608 926 8	0.665 907 19
	Bound 1	−4.335 424 1	3.656 644 5	0.428 858 20
	Bound 2	−5.379 404 1	4.903 083 9	0.573 176 69
	Exact	−5.734 014 6	4.694 394 3	0.669 477 54

This upper bound provides us with good results only at small temperatures, and moreover, it demands greater effort than the one needed by TDHA, as the sum in (25) must be performed numerically.

The bound (25) can be improved if one employs there the TDHA frequency $w(T)$ instead of the $T=0$ one of (24) [indeed the TDHA $w(T)$ almost coincides with the w value that one would obtain by minimizing (25) with respect to h]. Actually, the upper bound thus obtained is better than the TDHA one, as one includes now two-body terms in the density operator. This latest bound is not, however, easily dealt with in the case of more sophisticated $V(Q)$'s, as the evaluation of $\langle n \mid V(\hat{Q}) \mid n \rangle$ will not always constitute a light burden. One faces the computation of

$$\langle n \mid \hat{Q}^{2m} \mid n \rangle = \frac{(2m)!}{m!} h^m \sum_{1=0}^{m} 2^{-1} \begin{bmatrix} m \\ 1 \end{bmatrix} \begin{bmatrix} n \\ m-1 \end{bmatrix} , \qquad (26)$$

while the TDHA requires only working with a Laplace transform and just a single one-dimensional equation for the scaling parameter h. The TDHA does also away with any restrictions on the values that λ may adopt, opposite to what happens in the case of perturbative methods.

For future reference, the bound (25) will be referred to as bound 1, while the improvement to it mentioned in the preceding paragraph will be denoted as bound 2.

V. DISCUSSION AND CONCLUSIONS

Upper bounds to the free energy of the anharmonic oscillator have been studied, with particular emphasis on the one provided by the temperature-dependent Hartree approach. A very simple algorithm is introduced in order to deal with the TDHA, by appropriately generalizing the $T=0$ method of Ref. 5. The corresponding results have been compared, for the case $\lambda \hat{Q}^n$ with $n=4$ and 6, both to the exact ones and to the alternative bounds of Sec. IV. In the case $n=4$ we have also compared the results with the ones that arise out of Eq. (4) of Ref. 7 (see also Ref. 13). Our exact results were computed by (i) first performing a Hartree rotation of the SP basis (so as to minimize the ground-state energy) and (ii) diagonalizing $\hat{H}$ afterward in this undercomplete "dynamical" basis whose size is so chosen as to obtain convergence within eight significant digits. It is important to remark here that the corresponding eigenvalues coincide with the very accurate ones reported by Banerjee *et al.*,[14] which constitutes an excellent test for our calculations.

In Tables I and II, besides F, some additional quantities are also compared to the corresponding exact values, such as $E = \langle \hat{H} \rangle$ and the specific heat $C_v = T\partial S/\partial T$. The TDHA values can certainly be regarded as satisfactory ones, especially as regards E and Cv, and they improve with temperature. One of the two additional upper bounds introduced and discussed, constitutes an improvement upon the TDHA for computing F, but it does not provide one with a practical computational scheme for general types of potentials. Finally, a physically appealing picture of the TDHA in terms of scaling and "effective" wave functions is suggested.

ACKNOWLEDGMENT

The authors acknowledge support from the Argentine National Research Council (CONICET).

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