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Peculiarities of the Hartree approach to the temperature-dependent anharmonic oscillator

J Nuñez, A Plastino and R Rossignoli

Physics Department, National University, CC67, La Plata 1900, Argentina

Received 15 April 1987, in final form 7 September 1987

Abstract. With reference to the anharmonic oscillator problem, a temperature-dependent Hartree approach that is able to deal with quite general asymmetric potentials is presented. The mean-field approximation is seen to exhibit interesting phenomena associated with temperature changes.

1. Introduction

Interest in the one-dimensional anharmonic oscillator has been both sustained and intense in the past few decades, due mainly to its relevance for the study of molecular vibrations and to its role in the modelling of non-linear quantum field theories (for instance, Boyd 1978, Graffi and Grecchi 1973, Biswas *et al* 1973, Bender and Wu 1973, Lu *et al* 1973, Gillespie 1976, Bozzolo *et al* 1982, Flessas *et al* 1983, Chaudhuri and Mukherjee 1983, Znojil and Tater 1986).

A few years ago, a very elegant and powerful two-step approach to one-dimensional harmonic oscillators was introduced (Hsue and Chern 1984, hereafter referred to as I, Hsue 1986, Esebbag *et al* 1985), based upon a generalised coherent-state ansatz and a Bogoliubov transformation. This method can be shown to be equivalent to the Hartree approximation and has been generalised to the finite-temperature case (Nuñez *et al* 1986, hereafter referred to as II), but only with reference to some special situations, namely *even* potentials $V(x)$ that exhibit just one minimum. In such cases, the mean value of the coordinate x will vanish, and the Hartree mean field is governed by a single parameter: a temperature-dependent frequency. Changes either in the coupling constant (of $V(x)$) or in the temperature induce a smooth response from the Hartree field and no interesting phenomena are to be seen.

We wish here to generalise the work developed in II to a more general situation, allowing for potentials $V(x)$ that exhibit two or more minima. The concomitant physical problem becomes then a more interesting one. The mean value $\langle \hat{x} \rangle$ appears now as an additional variational parameter. Further, the self-consistent Hartree field may exhibit different behaviours for the diverse minima of $V(x)$, which may result in the appearance of various mean-field solutions and concomitant critical phenomena, as the temperature (or the coupling constant) changes. This fact, as far as we know, has not been stressed in recent literature (for instance, I).

It often happens, with regards to quite diverse physical contexts, that the appropriate Hartree (or Hartree-Fock) solution displays rather abrupt changes if some parameter of the system is modified, and one then speaks (more or less loosely) of phase transitions,

shape instabilities, etc, which are of considerable interest because they point towards possible instabilities of the corresponding solution. Thus, their study may provide one with valuable insights into the physics of the system under analysis. The present work attempts to perform a detailed study of the temperature-dependent anharmonic oscillator within this spirit in the hope that it may serve as a model for more complex situations.

A suitable generalisation of the formalism of II is represented in § 2. Application to a general anharmonic oscillator is dealt with in § 3, and two particularly interesting situations are considered, respectively, in §§ 4 and 5. The exact solution is also discussed in § 5, and some conclusions are drawn in § 6.

2. Formalism

We proceed here to generalise the formalism in II, so as to deal with quite general potentials $V(\hat{Q})$ that do not exhibit any particular symmetry. We start by defining 'unperturbed' (boson) creation and annihilation operators out of the coordinate \hat{Q} and the linear momentum \hat{P}

$$a^\dagger = (1/\sqrt{2})(\hat{Q} - i\hat{P}) \quad a = (1/\sqrt{2})(\hat{Q} + i\hat{P}) \quad (2.1)$$

in order to deal with Hamiltonians of the form

$$\hat{H} = \frac{1}{2}\hat{P}^2 + V(\hat{Q}). \quad (2.2)$$

We shall set both \hbar and Boltzmann's constant equal to unity and express the exact free energy as

$$F = \min_{\hat{\rho}_{\text{trial}}} T_r[\hat{\rho}_{\text{trial}}(\hat{H} - T\hat{S})] = -T \ln[T, \exp(-\beta\hat{H})] \quad (2.3)$$

where $\hat{S} = -\ln \hat{\rho}_{\text{trial}}$ is the so-called entropy operator and β is the inverse temperature ($\beta = 1/T$). The trial density matrix that minimises F is clearly the canonical one $\hat{\rho} = \exp(-\beta\hat{H})/T, \exp(-\beta\hat{H})$.

The central idea that underlies the Hartree scheme is that of working with a one-body density operator $\hat{\rho}$. Consequently, the temperature-dependent Hartree approximation (TDHA) for F will entail performing the minimisation of (2.3) within the set of one-body density operators

$$\hat{\rho} = \exp(\lambda_0 - w\beta b^\dagger b) \quad (2.4)$$

where b^\dagger and b are boson operators related to the 'unperturbed' ones (a^\dagger, a) by means of a general Bogoliubov transformation

$$b^\dagger = \alpha a^\dagger - \xi a + \gamma \quad b = \alpha^* a - \xi^* a^\dagger + \gamma^* \quad (2.5)$$

with $|\alpha|^2 - |\xi|^2 = 1$ so as to enforce boson commutation properties. 'New' canonical coordinates \hat{Q}' and \hat{P}' are associated to b^\dagger, b , namely

$$\begin{aligned} \hat{Q}' &= \text{Re}(\alpha - \xi^*)\hat{Q} + \text{Im}(\alpha - \xi^*)\hat{P} + \sqrt{2} \text{Re } \gamma \\ \hat{P}' &= \text{Re}(\alpha + \xi^*)\hat{P} - \text{Im}(\alpha + \xi^*)\hat{Q} - \sqrt{2} \text{Im } \gamma \end{aligned} \quad (2.6)$$

although, within the present context, α, ξ and γ may be assumed real, due to the structure of \hat{H} , which allows one to recast (2.6) as

$$\hat{Q}' = (\hat{Q} - q) e^{-h} \quad \hat{P}' = \hat{P} e^h \quad q = -\sqrt{2}\gamma e^h \quad \alpha = \cosh(h) \quad (2.7)$$

and one ascertains thus that the Bogoliubov transformation is merely a scaling transformation, with an appropriate translation.

Mean values of a given operator with respect to the density operator (2.4) can be easily obtained by recourse to Wick's theorem (Coleman 1975). The necessary ingredients are

$$f \equiv \langle b^\dagger b \rangle = T_r \hat{\rho} b^\dagger b = [\exp(\beta w) - 1]^{-1} \quad (2.8)$$

$$\langle b^\dagger \rangle = \langle b \rangle = \langle b^{\dagger 2} \rangle = \langle b^2 \rangle = 0 \quad (2.9a)$$

$$\langle \hat{Q} \rangle = \langle \hat{P} \rangle = 0 \quad (2.9b)$$

$$\langle \hat{Q}^2 \rangle = \langle \hat{P}^2 \rangle = f + \frac{1}{2}. \quad (2.9c)$$

In terms of the original operators some useful relationships are

$$\begin{aligned} \langle a^\dagger \rangle &= (1/\sqrt{2})q \\ \langle a^{\dagger 2} \rangle &= \frac{1}{2}q^2 + 2\alpha\xi(f + \frac{1}{2}) \\ \langle a^\dagger a \rangle &= \langle a^\dagger \rangle \langle a \rangle + \xi^2 + f(\alpha^2 + \xi^2) \\ \langle \hat{Q} \rangle &= q \\ \langle \hat{P} \rangle &= 0 \\ \langle \hat{Q}^2 \rangle &= q^2 + G^2 \\ \langle \hat{P}^2 \rangle &= (f + \frac{1}{2})^2 / G^2 \\ G^2 &= \langle \hat{Q}^2 \rangle - q^2 = e^{2h}(f + \frac{1}{2}) \end{aligned} \quad (2.10)$$

and, finally,

$$\langle V(\hat{Q}) \rangle = \left(\frac{1}{4\pi t} \right)^{1/2} \int_{-\infty}^{\infty} \exp[-(x - q)^2/4t] V(x) dx \quad t = \frac{1}{2}G^2 \quad (2.11)$$

which represents a displaced Gaussian distribution. Of special interest is the case $V(\hat{Q}) = \hat{Q}^n$

$$\langle \hat{Q}^n \rangle = \sum_{m=0}^{[n/2]} \frac{n! q^{(n-2m)} G^{2m}}{(n-2m)! m! 2^m}. \quad (2.12)$$

In order to evaluate the Hartree free energy we also need the entropy, which is given by the well known single-particle expression

$$S = -T_r \hat{\rho} \ln \hat{\rho} = -[f \ln f - (f + 1) \ln (f + 1)] \quad (2.13)$$

in terms of the Bose occupation number (2.8). The TDHA equations are now obtained by requiring that $F = \langle \hat{H} \rangle - T \langle \hat{S} \rangle$ be stationary with respect to w (cf (2.4)), γ (cf (2.5)) and h (cf (2.6)). An alternative set of independent variables is given by f , G and q . Minimisation with respect to f is immediately performed (see II), and one obtains

$$w = (f + \frac{1}{2}) / G^2 = e^{-2h} \quad (2.14a)$$

or, alternatively,

$$f = \{ \exp[\beta(f + \frac{1}{2}) / G^2] - 1 \}^{-1} \quad (2.14b)$$

so that one is finally led to the set of equations

$$\frac{\partial F}{\partial q} = \frac{\partial}{\partial q} \langle V(\hat{Q}) \rangle = 0 \quad \frac{\partial F}{\partial G^2} = \frac{\partial}{\partial G^2} \langle V(\hat{Q}) \rangle - \frac{(f + \frac{1}{2})^2}{2G^4} = 0 \quad (2.15)$$

which, when properly solved, provide us with an upper bound to the exact free energy.

The Hartree expression for the specific heat $C_v = T \partial S / \partial T$ is given by

$$C_v = T \ln \left(\frac{f+1}{f} \right) \frac{df}{dT}. \quad (2.16)$$

Notice that the values of G^2 , q and f that minimise F depend upon the temperature. Of course, the occupation number f , together with S , vanishes at $T = 0$.

3. An anharmonic potential

Let us tackle first the case of an anharmonic potential, whose Hamiltonian is

$$\begin{aligned} \hat{H} &= \frac{1}{2} \hat{P}^2 + V(\hat{Q}) \\ &= \frac{1}{2} (\hat{P}^2 + K \hat{Q}^2) + \delta \hat{Q}^3 + \lambda \hat{Q}^4 \\ &= \lambda^{1/3} [\frac{1}{2} (\hat{P}'^2 + K' \hat{Q}'^2) + \delta' \hat{Q}'^3 + \hat{Q}'^4] \end{aligned} \quad (3.1)$$

with $\hat{P}' = \lambda^{-1/6} \hat{P}$, $\hat{Q}' = \lambda^{1/6} \hat{Q}$, $\delta' = \lambda^{-5/6} \delta$ and $K' = \lambda^{-2/3} K$, $\lambda > 0$, the coordinates corresponding to a system with the origin located at the bottom of the potential (if $K > 0$). The potential $V(\hat{Q})$ exhibits three extrema for $K < 9\delta^2/16\lambda$ (two minima and a maximum) and just a single minimum otherwise.

Recourse to (2.11)–(2.15) yields the following results (we set $r \equiv G^2$)

$$\langle \hat{H} \rangle = \frac{1}{2} [(f + \frac{1}{2})^2 / r + K(r + q^2)] + \delta(q^3 + 3rq) + \lambda(q^4 + 6q^2r + 3r^2) \quad (3.2)$$

$$\partial F / \partial q = Kq + 3\delta(q^2 + r) + 4\lambda(q^3 + 3qr) = 0 \quad (3.3a)$$

$$\partial F / \partial r = \frac{1}{2} [K - (f + \frac{1}{2})^2 / r^2] + 3\delta q + 6\lambda(q^2 + r) = 0 \quad (3.3b)$$

which leads to

$$r = -(Kq + 4\lambda q^3 + 3\delta q^2) / (12\lambda q + 3\delta) \quad (3.4)$$

$$(f + \frac{1}{2})^2 = r^2 (K + 12\lambda q^2 + 6\delta q) + 12\lambda r^3 \quad (3.5)$$

so that just a single equation is to be solved, namely (2.14b) with f and r being expressed in terms of the displacement q by means of (3.4) and (3.5). According to the relative values of λ , δ and K , several roots may arise out of (2.14). Two specific situations will be discussed in the following two sections.

In the classical limit, $T \rightarrow \infty$, the TDHA yields the correct leading terms in the asymptotic expressions of thermodynamic quantities (cf II). Since in the high-temperature region the behaviour of our system is governed by the quartic term, the asymptotic expressions presented in II remain valid within the present context, save for the translation q ,

$$q = \langle \hat{Q} \rangle \xrightarrow{T \rightarrow \infty} \frac{\delta}{4\lambda} \left(-1 + \frac{K - \delta^2/2\lambda}{(12\lambda T)^{1/2}} \right). \quad (3.6)$$

As $\lambda \hat{Q}^4 + \delta \hat{Q}^3$ equals $\lambda (\hat{Q} + \delta/4\lambda)^4$ plus quadratic, linear and constant terms whose influence vanishes for T high enough, the meaning of the factor $\delta/4\lambda$ in (3.6) becomes transparent.

4. The bistable potential

This situation arises when the potential exhibits two minima of equal depth. This will happen whenever (a) $K < 0$ and $\delta = 0$ or (b) $K = \delta^2/2\lambda$. In both cases we deal with a symmetric potential (around the origin or around $-\delta/4\lambda$, respectively). For case (a) (3.3) become

$$q[K + 4\lambda(q^2 + 3r)] = 0 \quad (f + \frac{1}{2})^2 - r^2[12\lambda(r + q^2) + K] = 0 \quad (4.1)$$

so that a symmetric (that is, with $q = 0$) solution will always exist. However, a symmetry-breaking (sb) degenerate solution is also feasible, for

$$q = \pm(-K/4\lambda - 3r)^{1/2} \quad (4.2)$$

and r a root of

$$(f + \frac{1}{2})^2 + 2r^2(12\lambda r + K) = 0 \quad (4.3)$$

where f satisfies (2.14). Real, positive solutions of (4.3) exist only for $-K > (486)^{1/3}[(f + \frac{1}{2})\lambda]^{2/3}$. Thus, at zero temperature ($f = 0$), the sb solution exists if

$$K < K_c(T = 0) \equiv K_0 \equiv -(243/2)^{1/3}\lambda^{2/3}. \quad (4.4)$$

In this case, five TDHA stationary solutions can be found, namely, two degenerate minima, two degenerate saddle points and a minimum at $q = 0$. For $K > K_c$, only one minimum remains (at $q = 0$).

When comparing the displaced minimum ($q \neq 0$) with the symmetric one ($q = 0$), the former lies deeper for $K < K'_0 \equiv 1.084\,906\,K_0$. Thus, there is a narrow range of K values for which both solutions exist but the symmetric one prevails. At $K = K'_0$ a first-order phase transition takes place, with abrupt changes both in r and q . This phase transition reflects the fact that, in the exact ground state, the peak of the density $\rho(Q) = \langle Q | \hat{\rho}_{\text{exact}} | Q \rangle$ changes from zero up to a degenerate maximum, within the range $1.3K_0 < K < 0.75K_0$, although without undergoing any sudden change.

For fixed values of K similar behaviours are to be observed as the temperature grows. The sb solution exists for $T < T_c(K)$ (or equivalently, $K < K_c(T) < K_0$) and yields the lowest free energy for $T < T'_c(K) < T_c(K)$ (or $K < K'_c(T) < K_c(T)$). A first-order transition occurs at $T = T'_c(K)$ from the sb to the symmetric solution as T increases. However, this transition does not correspond to a change in the peak of the exact density, but to a 'flattening' of this density. One should recall that the classical density is proportional to $\exp(-\beta V(Q))$ and that classical behaviour should be observed for high enough temperatures. This behaviour is properly matched by the TDHA as it becomes symmetric once again at the critical temperature.

Some typical results are displayed in table 1. The sb solution is quite good as far as the mean energy is concerned. Whenever the temperature lies within the metastable region ($T'_c < T < T_c$), the sb solution compares favourably to the symmetric one, if one focuses attention upon the $\langle \hat{H} \rangle$ values. However, as the latter allows for a better estimate of the entropy, it yields a lower free energy. The asymmetric character of the sb solution (involving a greater degree of 'order') explains the poor entropy estimation. A better (larger) entropy would be obtained by restoring the symmetry with a density operator of the form $\hat{\rho}_s = \frac{1}{2}[\hat{\rho}_d(q) + \hat{\rho}_d(-q)]$, due to the well known concavity property of S ($\hat{\rho}_d$ stands for the displaced Hartree density operator).

Table 1. Quantities of interest for the bistable potential as a function of the temperature T . (a) Exact results; (b) symmetry-breaking (sb) solution; (c) symmetric solution. The parameters of the potential are $\lambda = 1.0$ and $K = 1.5K_0$. Solution (c) is lower than (b) for $T > T'_c = 1.398$. At $T = T_c = 2.008$ the sb solution ceases to exist.

T	F	$\langle \hat{H} \rangle$	S	C_0	$\langle \hat{Q}^2 \rangle$	$\langle \hat{Q} \rangle$	
(a)	-1.761 38	-1.761 38	0	0	1.441 11	0	
(b)	0	-1.637 00	0	0	1.559 68	1.187 79	
(c)	-0.955 61	-0.955 61	0	0	0.666 07	0	
(a)	-1.972 77	-1.698 08	0.686 75	0.084 28	1.525 28	0	
(b)	0.4	-1.637 09	-1.636 24	0.002 12	0.031 66	1.559 52	1.187 69
(c)	-1.008 86	-0.858 24	0.376 55	0.816 87	0.686 59	0	
(a)	-2.270 94	-1.615 58	0.819 20	0.338 76	1.522 54	0	
(b)	0.8	-1.649 24	-1.584 67	0.080 72	0.482 69	1.548 55	1.180 74
(c)	-1.237 41	-0.651 21	0.732 76	0.800 71	0.725 79	0	
(a)	-2.633 58	-1.440 70	0.994 06	0.514 09	1.508 03	0	
(b)	1.2	-1.715 28	-1.403 75	0.259 60	0.774 30	1.508 05	1.154 74
(c)	-1.578 21	-0.428 98	0.957 69	0.767 73	0.763 01	0	
(a)	-2.840 79	-1.332 84	1.077 11	0.561 20	1.501 85	0	
(b)	1.4	-1.777 64	-1.266 51	0.365 10	0.824 58	1.474 87	1.132 98
(c)	-1.778 75	-0.314 82	1.045 67	0.755 99	0.780 67	0	
(a)	-3.302 06	-1.096 80	1.225 14	0.611 88	1.494 41	0	
(b)	1.8	-1.968 95	-0.892 86	0.597 83	0.862 72	1.368 36	1.060 13
(c)	-2.227 37	-0.082 04	1.191 85	0.739 09	0.814 29	0	
(a)	-3.553 69	-0.973 02	1.290 34	0.624 99	1.493 19	0	
(b)	2.0	-2.103 15	-0.572 61	0.765 27	0.913 23	1.236 96	0.962 69
(c)	-2.472 06	-0.036 19	1.254 13	0.732 95	0.830 32	0	
(a)	-4.093 52	-0.719 74	1.405 74	0.639 47	1.495 08	0	
(b)	2.4	—	—	—	—	—	
(c)	-2.996 15	0.275 71	1.363 27	0.723 72	0.861 06	0	

5. Effects of a cubic term

If we add now a (small) cubic term to the preceding bistable potential, the two former minima cease to exhibit an identical depth. Consequently, the previous degeneracy of the displaced Hartree solutions is removed, and the minimum that existed at the origin will be shifted to a different location. The interest of the problem lies now in the fact that if the parameter δ in (3.1) starts to grow, new critical phenomena become apparent.

Let us concentrate our attention upon the situation illustrated in table 1, namely the particular case $K = 1.5K_0$. For δ small enough, the overall picture is that of the former section. First-order corrections (in δ) to the coordinate q are

$$q_0 = \frac{-3\delta r_0}{12\lambda r_0 + K} \quad q_d = \pm \left(\frac{-K - 12\lambda r_d}{4\lambda} \right)^{1/2} - \frac{3\delta(r_0 + K/16\lambda)}{K + 12\lambda r_d} \quad (5.1)$$

where the subscript 0 refers to the symmetric solution and the subscript d to the sb one. The three minima 'move' towards the location of the deepest minimum of $V(Q)$, whereas the two saddle points are displaced in the opposite direction. Now at $T=0$,

when $\delta \approx \pm 0.0375$, one of the minima and one of the saddle points disappear, and we are left with two minima (located in the vicinity of the corresponding wells) and a saddle point. At $\delta \approx \pm 0.9095$, just a single TDHA solution remains, corresponding to the deepest well (the shallow one exhibits, for this value of δ , a depth of about 26.6% of that corresponding to the deepest well).

The behaviour of the system for fixed values of δ and K as T grows is illustrated in table 2 and figure 1, for the case $\delta = -0.1$. A 'near-symmetric' (NS) solution, not present at $T=0$, appears at $T = T_c \approx 0.675$ (together with a saddle point), becoming the deepest one at $T = T_{c2} \approx 1.704$. All the remaining solutions disappear for sufficiently high T . This NS solution exhibits a lower degree of order than the displaced ones, i.e. a larger fluctuation and a greater entropy, which accounts for the lower free energy, although its mean-energy prediction is poor. In order to interpret the meaning of these TDHA transitions, it may be helpful to look at the behaviour of the exact $\langle \hat{Q} \rangle$ values, illustrated in figure 2, which undergo a rapid decrease for small T .

Table 2. Same quantities as in table 1 but for the potential $V(x) = \frac{1}{2}Kx^2 + \delta x^3 + \lambda x^4$, with $\lambda = 1.0$, $\delta = -0.1$ and $K = 1.5K_0$. (a) Exact results; (b) 'displaced' solution; (c) 'near symmetric' solution; (d) 'shallow-minimum' solution. At $T=0$, (e) refers to the first excited state (see text).

T	F	$\langle \hat{H} \rangle$	S	C_v	$\langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2$	$\langle \hat{Q} \rangle$
(a)	-1.927 27	-1.927 27	0	0	0.282 99	1.154 74
(b)	-1.868 02	-1.868 02	0	0	0.145 26	1.234 08
(c)	—	—	—	—	—	—
(d)	-1.426 25	-1.426 25	0	0	0.152 62	-1.141 85
(e)	-1.470 47	-1.470 47	0	0	0.370 98	-1.051 92
(a)	-2.163 42	-1.755 58	0.679 74	0.314 35	1.365 50	0.449 20
(b)	-1.869 93	-1.856 82	0.021 91	0.206 16	0.146 36	1.232 72
(c)	—	—	—	—	—	—
(d)	-1.428 82	-1.412 13	0.027 82	0.244 83	0.154 22	-1.139 76
(a)	-2.390 47	-1.640 84	0.832 92	0.450 10	1.445 89	0.317 58
(b)	-1.888 18	-1.789 13	0.110 06	0.566 45	0.153 15	1.224 38
(c)	-1.332 02	-0.625 53	0.784 99	0.799 51	0.717 50	0.172 49
(d)	-1.450 72	-1.334 37	0.129 28	0.610 09	0.163 22	-1.127 93
(a)	-2.975 06	-1.316 96	1.105 40	0.600 23	1.474 91	0.203 46
(b)	-2.035 96	-1.443 45	0.395 01	0.832 25	0.190 71	1.177 13
(c)	-1.899 18	-0.277 22	1.081 31	0.754 67	0.782 72	0.118 36
(d)	-1.619 84	-0.943 52	0.450 88	0.845 01	0.215 32	-1.056 81
(a)	-3.323 89	-1.132 34	1.217 53	0.628 23	1.478 14	0.174 29
(b)	-2.178 37	-1.177 56	0.556 00	0.855 34	0.224 12	1.133 50
(c)	-2.240 18	-0.100 03	1.188 97	0.741 83	0.809 60	0.105 65
(d)	-1.785 78	-0.562 34	0.679 69	0.894 04	0.289 41	-0.946 16
(a)	-3.704 15	-0.941 77	1.315 42	0.641 38	1.481 54	0.153 49
(b)	-2.371 49	-0.819 93	0.738 84	0.880 40	0.279 92	1.056 71
(c)	-2.611 02	0.079 22	1.281 07	0.732 46	0.834 65	0.096 50
(d)	—	—	—	—	—	—
(a)	-4.111 96	-0.748 19	1.401 60	0.648 39	1.486 19	0.137 98
(b)	—	—	—	—	—	—
(c)	-3.007 68	-0.260 36	1.361 68	0.725 46	0.858 32	0.089 54
(d)	—	—	—	—	—	—

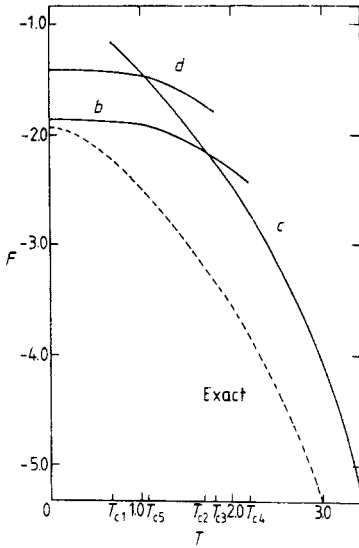


Figure 1. Free energies corresponding to the different solutions of (3.3) (full curves), and exact results, for the potential with the cubic term. The parameters are the same as those in table 2. Critical temperatures are indicated. T_{c2} and T_{c3} indicate 'level crossing'. T_{c1} is that temperature at which the symmetric solution appears for the first time. T_{c3} and T_{c4} , on the other hand, are the critical temperatures above which the corresponding solution ceases to exist. For the meaning of (b), (c), (d) see table 2.

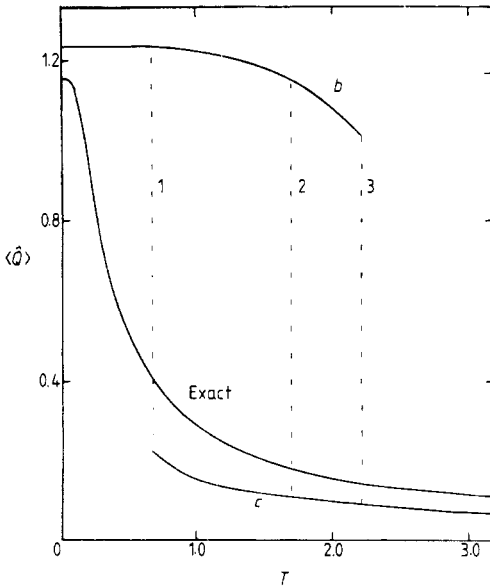


Figure 2. Mean value of the coordinate against T , according to the Hartree solutions (b) and (c), and exact values, for the Hamiltonian of table 2. The vertical broken lines indicate mean-field 'phase transitions' according to the maximum entropy (1), minimum free energy (2), and minimum energy (3) criteria.

The former behaviour occurs for $0.0375 < |\delta| < 1.02$. For higher values of δ , the NS solution does not reappear at finite T , and the evolution of the system (as T grows) becomes smooth in TDHA.

The metastable TDHA solution corresponding to the shallow well can be regarded at $T = 0$ as an approximation to the first excited state of \hat{H} . At finite T , TDHA depicts approximately the evolution of this metastable configuration, which disappears for $T > T_{c3}$.

The TDHA prediction for the specific heat is in general poor at low temperatures, but results improve as T grows.

The exact eigenvalues and eigenfunctions of (3.1) have been computed according to the procedures discussed in I, i.e. the diagonalisation of \hat{H} in an optimised Hartree basis. However, since several Hartree solutions may exist at $T = 0$, the question of which one yields the fastest convergence arises. In general, the deepest Hartree solution is the best as regards the ground state. But it may not be so for other levels.

For instance, in the cubic case discussed in table 2, a 20×20 diagonalisation with the deepest $T = 0$ Hartree basis yields the best estimate for the ground state. Indeed, using the Hartree basis centred around the shallow minimum yields a very good value for the first excited state and, in addition, better figures for the first few levels (see table 3). With a 40×40 diagonalisation, however, all differences vanish, and both solutions yield exact values for the first nine levels up to eight significant digits.

Table 3. Lowest lying levels for the Hamiltonian of table 2, for various dimensions of the corresponding energy matrix and different Hartree basis: (b) indicates that corresponding to the deepest $T = 0$ Hartree solution, while (d) refers to the basis centred around the shallow minimum.

	10 × 10		20 × 20		30 × 30		40 × 40
	(b)	(d)	(b)	(d)	(b)	(d)	(b), (d)
E_0	-1.920 0907	-1.492 1396	-1.926 9317	-1.921 2578	-1.927 2677	-1.927 2671	-1.927 2677
E_1	0.308 8737	0.077 1951	-1.440 9766	-1.470 0670	-1.470 4705	-1.470 4708	-1.470 4708
E_2	1.878 0254	1.843 4449	0.669 4388	0.655 0543	0.639 9225	0.639 9237	0.639 9220
E_3	4.747 6714	4.622 1944	2.151 9007	2.082 4597	2.042 1451	2.042 1468	2.042 1422
E_4	8.215 4376	7.991 8896	4.388 1601	4.263 7932	4.150 1208	4.150 1192	4.150 1058

6. Conclusions

We have shown in this paper that a simple generalisation of the TDHA formalism presented in II enables the mean-field approach to deal with situations in which the potential exhibits several extrema, or with general asymmetric potentials. The new ingredient is found to be the inclusion, within the formalism, of the translation $\langle \hat{Q} \rangle$ as a variational parameter.

In this way, even a quartic anharmonic oscillator with a cubic term displays critical behaviour in the mean-field approach. The accuracy of the mean-field approximation decreases in the critical regions. The Hartree phase transitions can be associated with significant (although not sudden) changes in the structure of the exact solution.

It is also of interest to point out that the existence of metastable Hartree solutions at finite temperatures can be connected to metastable situations that arise in an exact description (for an illustration of this feature that is found in nuclear physics see Miller *et al* 1986).

As a final remark, the importance of finding self-consistent Hartree solutions lies in the fact that they constitute a good (undercomplete) basis for configuration mixing improvements (at $T=0$) or for those that are achieved by linear combinations of density matrices (at $T \neq 0$).

Acknowledgment

The authors are indebted to the National Research Council of Argentina (CONICET) for its support.

References

- Bender C and Wu T T 1973 *Phys. Rev. D* **7** 1670
 Biswas S N, Datta K, Saxena R P, Srivastava P K and Varma V S 1973 *J. Math. Phys.* **14** 1190
 Boyd J P 1978 *J. Math. Phys.* **19** 1445
 Bozzolo G, Esebbag C and Plastino A 1982 *Phys. Rev. D* **26** 801
 Chaudhuri R N and Mukherjee B 1983 *J. Phys. A: Math. Gen.* **16** 3193
 Coleman S 1975 *Phys. Rev. D* **11** 2088
 Esebbag C, Nuñez J, Plastino A and Bozzolo G 1985 *Phys. Rev. D* **32** 522
 Flessas G P, Whitehead R R and Rigas A 1983 *J. Phys. A: Math. Gen.* **16** 85
 Gillespie G H 1976 *Lett. Nuovo Cimento* **16** 86
 Graffi S and Grecchi V 1973 *Phys. Rev. D* **8** 3487
 Hsue C S 1986 *Phys. Rev. A* **33** 1392
 Hsue C S and Chern J L 1984 *Phys. Rev. D* **29** 643
 Lu P, Wald S S and Young B L 1973 *Phys. Rev. D* **7** 1701
 Miller H G, Quick R M, Bozzolo G and Vary J P 1986 *Phys. Lett.* **168B** 13
 Nuñez J, Plastino A and Rossignoli R 1986 *Phys. Rev. D* **33** 1709
 Znojil M and Tater M 1986 *J. Phys. A: Math. Gen.* **19** 2317