Convexity property of the variational approximations to the effective potential

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The convexity property of the variational approximations to the effective potential is analyzed both in quantum mechanics and in $\lambda\phi^4$ field theory. A simple calculational scheme, based on the generalization of the Gaussian functionals subspace, allows one to reproduce this fundamental feature of the exact effective potential to a very high degree of accuracy. A criterion to clarify the occurrence of spontaneous symmetry breaking in the presence of a flat effective potential is proposed.

I. INTRODUCTION

Effective-potential techniques are very useful tools to investigate the occurrence of nonperturbative phenomena, such as spontaneous symmetry breaking, both in quantum mechanics and quantum field theory. Two basically different approaches to the calculation of the effective potential exist. The first one, based on a semiclassical approximation, the loop expansion,[1] can be applied in the presence of classically stable configurations and in a situation where quantum fluctuations are "small." This approach, essentially of perturbative nature, does not enjoy any stability property. As shown in Ref. 2 for $\lambda\phi^4$ theory and in Ref. 3 for Yang-Mills theories, the one-loop effective potential is obtained by minimizing the expectation value of the shifted, linearized Hamiltonian in a Gaussian state. Now, the linearized Hamiltonian may exhibit well-known pathologies, such as unboundedness from below, which show up in the appearance of unphysical imaginary parts, and there is no guarantee, in principle, that, by increasing the accuracy in $\hbar$, one also gets a better estimate of the ground-state energy.

The above arguments suggest that the second approach, based on the variational method, is clearly advantageous and necessary in those cases in which quantum fluctuations can sizably change the naive expectations based on the classical potential. Clearly, in this second framework, both the estimate of the ground-state energy and the general validity of the various statements concerning the occurrence of the spontaneous symmetry breaking strongly depend on the subspace explored in the variational procedure. For instance, as discussed in Refs. 4 and 5, in the Gaussian approximation, spontaneous symmetry breaking is discovered as a sensible phenomenon in pure $\lambda\phi^4$ theory.[6] The statement, being of variational nature, implies that, within the subspace of normalized Gaussian states, the symmetric state with $\langle\phi\rangle=0$, the perturbative vacuum, is not the lowest.

No definite statement, however, can be drawn concerning the possible existence of symmetric, non-Gaussian states of still lower energy. In particular the property of the exact effective potential, its convexity,[7–14] is not recovered in its Gaussian approximation. The question then naturally arises of finding variational approximations that enjoy this fundamental property and, at the same time, allow one to understand spontaneous symmetry breaking.

In this paper we shall address, in Sec. II, the question of the convexity of the variational approximations to the effective potential in the case of the double-well potential of quantum mechanics. In Sec. III we shall discuss the case of quantum field theory.

II. DOUBLE-WELL POTENTIAL

In this section we shall consider the quantum anharmonic oscillator whose Hamiltonian is

$$\hat{H}=\frac{\hat{p}^2}{2m}-\tfrac{1}{2}|k|\hat{x}^2+\frac{\lambda}{4!}\hat{x}^4 , \tag{2.1}$$

with $\lambda>0$. The effective potential is defined as

$$V(\bar{x})=\min_{[\psi]}\langle\psi|\hat{H}|\psi\rangle , \tag{2.2}$$

where $[\psi]$ is the set of normalized quantum states for which

$$\langle\psi|\hat{x}|\psi\rangle=\bar{x} . \tag{2.3}$$

We shall (i) summarize the main features of the single-Gaussian approximation to the effective potential, then (ii) discuss the results obtained by using, as a trial state, the linear superposition of two Gaussian wave functions.

A. Single Gaussian

In this approximation we calculate the energy expectation value among the normalized Gaussian functions

$$\psi(x)=\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\sigma}}\exp\left[-\frac{(x-\bar{x})^2}{2\sigma^2}\right] , \tag{2.4}$$

which satisfy Eq. (2.3); they depend on two variational parameters $\bar{x}$ and σ, so we have

$$\langle\psi|\hat{H}|\psi\rangle=E(\bar{x},\sigma) . \tag{2.5}$$

Introducing the dimensionless variables

$$f=\bar{x}\left[\frac{\lambda}{|k|}\right]^{1/2},$$
$$g=\frac{\hbar}{\sigma^2}\left[\frac{1}{m|k|}\right]^{1/2}, \qquad (2.6)$$
$$\epsilon=\frac{\lambda\hbar}{|k|^{3/2}m^{1/2}},$$

we have

$$E(\bar{x},\sigma)=\frac{k^2}{\lambda}Z(f,g), \qquad (2.7)$$

where

$$Z(f,g)=\frac{\epsilon g}{4}-\frac{1}{2}f^2+\frac{1}{24}f^4-\frac{\epsilon}{4g}(1-\tfrac{1}{2}f^2)+\frac{\epsilon^2}{32g^2}. \qquad (2.8)$$

The Gaussian effective potential is obtained by minimizing $Z(f,g)$ with respect to g. From the equation $\partial Z/\partial g=0$ we get

$$g^2=-1+\tfrac{1}{2}f^2+\frac{\epsilon}{4g} \qquad (2.9)$$

and setting $g(f)$ as the solution of the Eq. (2.9), we define

$$V_G\left[\left[\frac{|k|}{\lambda}\right]^{1/2}f\right]=Z(f,g(f))\frac{k^2}{\lambda}. \qquad (2.10)$$

By using Eq. (2.9) we find

$$\frac{dV_G}{df}=f[g^2(f)-\tfrac{1}{3}f^2]\frac{k^2}{\lambda}. \qquad (2.11)$$

From this derivative we see that V_G has extrema at

$$f=0 \qquad (2.12)$$

and at those values $\bar{f}$ for which

$$g^2(\bar{f})=\tfrac{1}{3}\bar{f}^2. \qquad (2.13)$$

The equation for $\bar{f}$ can be written, using again Eq. (2.9),

$$-1+\tfrac{1}{6}\bar{f}^2+\frac{\sqrt{3}}{4}\frac{\epsilon}{|\bar{f}|}=0, \qquad (2.14)$$

and the value of $Z(f)$ at $f=\bar{f}$ is

$$Z(\bar{f})=-\tfrac{1}{2}+\tfrac{1}{3}|\bar{f}|^2-\tfrac{1}{12}|\bar{f}|^4. \qquad (2.15)$$

We can easily get solutions of Eq. (2.14) for small ϵ:

$$|\bar{f}|_M=|O(\epsilon)|,$$
$$|\bar{f}|_m=\sqrt{6}-|O(\epsilon)|. \qquad (2.16)$$

The values of $Z(f)$ at the extrema (2.12) and (2.16),

$$Z(|\bar{f}|_m)=-\tfrac{3}{2}+|O(\epsilon)|,$$
$$Z(|\bar{f}|_M)>Z(0)=-\tfrac{1}{2}+|O(\epsilon)|, \qquad (2.17)$$

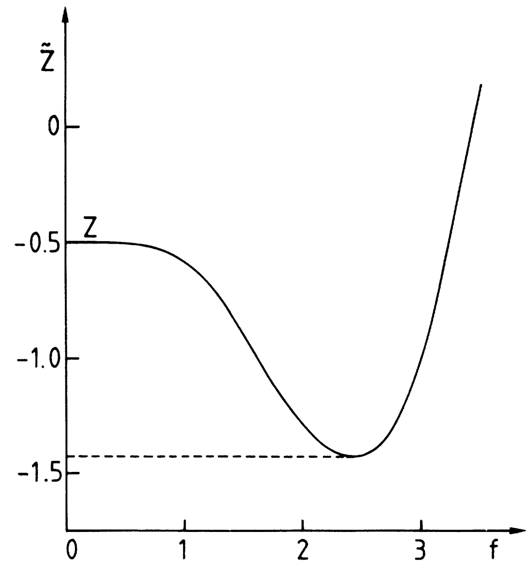

FIG. 1. The symmetrical functions $Z(f)$ (solid line) and $\tilde{Z}(f)$ (dashed line) are plotted at $\epsilon=0.1$ for positive f. Beyond the minimum of $Z(f)$ the two functions become equal.

show that the Gaussian potential in the weak-coupling limit ($\epsilon \ll 1$) has two nonsymmetrical absolute minima at $\pm|\bar{f}|_m$ located near the minima of the classical potential set in a dimensionless form ($|\bar{f}|_c=\pm\sqrt{6}$), while $f=0$ and $\pm|\bar{f}|_M$ are a local minimum and local maxima, respectively.

We notice that in the weak-coupling regime the single-Gaussian approximation to the effective potential gives, at the absolute minima, a reliable value of the ground-state energy. This happens since the shift of the energy levels in the two wells due to the tunneling is exponentially small:

$$\left|\frac{\Delta E}{E}\right|\sim\exp\left[-\frac{1}{\epsilon}\right]. \qquad (2.18)$$

However the single-Gaussian approximation, at least for small ϵ, does not enjoy the fundamental property of convexity for each value of $\bar{x}$ (see Fig. 1).

B. Double Gaussian

A natural way to go beyond the single-Gaussian results is to consider, as a trial wave function, the superposition

$$\tilde{\psi}(x)=\alpha_1\psi_1(x,\sigma_1,\bar{x}_1)+\alpha_2\psi_2(x,\sigma_2,\bar{x}_2), \qquad (2.19)$$

where ψ_1 and ψ_2 have the form of (2.4) and α_1 and α_2 are real parameters. The energy expectation value, using again Eqs. (2.6), is now

$$E(f_1,f_2,g_1,g_2,\alpha_1,\alpha_2)=\frac{k^2}{\lambda}\left[\alpha_1^2 Z(f_1,g_1)+\alpha_2^2 Z(f_2,g_2)+\frac{\alpha_1\alpha_2 T}{g_1+g_2}\left[\epsilon g_1 g_2(1-\tau)-\epsilon-\chi+\frac{3\epsilon^2+6\epsilon\chi+\chi^2}{12(g_1+g_2)}\right]\right], \tag{2.20}$$

where

$$\tau=\frac{g_1g_2}{g_1+g_2}\frac{(f_1-f_2)^2}{\epsilon},$$
$$\chi=\frac{(f_1g_1+f_2g_2)^2}{g_1+g_2}, \tag{2.21}$$
$$T=\langle\psi_1|\psi_2\rangle=\left[\frac{2\sqrt{g_1g_2}}{g_1+g_2}\right]^{1/2}\exp\left[-\frac{\tau}{2}\right].$$

Now we have to optimize six variational parameters, but we can eliminate one of them (α_2) by using the normalization condition for $\tilde{\psi}(x)$:

$$\alpha_1^2+\alpha_2^2+2\alpha_1\alpha_2 T=1 . \tag{2.22}$$

Moreover we want to express the effective potential uniquely as a function of $\bar{x}$, the coordinate expectation value for $\tilde{\psi}(x)$. Since in our case it is

$$f=\langle\tilde{\psi}|\hat{x}|\tilde{\psi}\rangle\left[\frac{\lambda}{|k|}\right]^{1/2}$$
$$=\tfrac{1}{2}y+\frac{w}{2}\left[\alpha_1^2-\alpha_2^2+\frac{g_1-g_2}{g_1+g_2}(1-\alpha_1^2-\alpha_1^2)\right], \tag{2.23}$$

with

$$w=f_1-f_2,$$
$$y=f_1+f_2,$$

we can use Eqs. (2.22) and (2.23) to write

$$\langle\tilde{\psi}|\hat{H}|\tilde{\psi}\rangle=\frac{k^2}{\lambda}\tilde{Z}(f,w,g_1,g_2,\alpha_1) . \tag{2.24}$$

From Eqs. (2.20) and (2.23) follows that $\tilde{Z}$ is symmetrical in the sense that if, with f fixed ($f=f^*$), we get a minimum of $\tilde{Z}$ for the configuration $[f_1^*,f_2^*,g_1^*,g_2^*,\alpha_1^*,\alpha_2^*]$, then, at $f=-f^*$, we obtain the same value of $\tilde{Z}$ for $[-f_2^*,-f_1^*,g_2^*,g_1^*,\alpha_2^*,\alpha_1^*]$.

We obtain the effective potential $V_{DG}(f)$ in this approximation by a numerical minimization of $\tilde{Z}$ with respect to w,g_1g_2,α_1, keeping fixed f:

$$V_{DG}(f)=\frac{k^2}{\lambda}\tilde{Z}(f,w(f),g_1(f),g_2(f),\alpha_1(f)) . \tag{2.25}$$

For small ϵ, V_{DG} is convex since it has a single well shape with a flat central region. In Fig. 1 $\tilde{Z}(f)$, for $\epsilon=0.1$, is shown. In this case we find the value

$$\tilde{Z}=-1.429\,604\,634\,009(693)$$

with the interval

$$-2.427\,545\,935\,4(337)<f<2.427\,545\,935\,4(337) .$$

The weak-coupling analysis performed so far shows that, to a very high accuracy, the exact effective potential can be reproduced by exploring our limited subspace. The effective potential, in this regime, is flat within the region enclosed by the classical minima, the energy gain due to the tunneling being exponentially small. Strictly speaking, the absolute minimum should be at $\bar{x}=0$ but the difference is out of reach of our numerical analysis. In this sense one can conclude that there is no spontaneous symmetry breaking; however, our analysis of an almost flat effective potential could have some relevance in the quantum-field-theoretical case where, as we shall see in Sec. III, the effective potential is exactly flat in the infinite-volume limit, and one needs some further indications to understand, in this case, the occurrence of spontaneous symmetry breaking.

Indeed a simple argument to weight degenerate quantum states is to calculate the density probability for the various configurations. In our case one has to compute

$$W(\bar{x})=|\tilde{\psi}_{\bar{x}}(\bar{x})|^2 , \tag{2.26}$$

where $\tilde{\psi}_{\bar{x}}(x)$ is the optimal wave function at which

$$V_{DG}(\bar{x})=\langle\tilde{\psi}_{\bar{x}}|\hat{H}|\tilde{\psi}_{\bar{x}}\rangle \tag{2.27}$$

and

$$\bar{x}=\langle\tilde{\psi}_{\bar{x}}|\hat{x}|\tilde{\psi}_{\bar{x}}\rangle . \tag{2.28}$$

The above procedure is the variational counterpart of the intuitive statement that in the weak-coupling regime ($\epsilon\ll 1$), the system possesses two very different time scales, exponentially $[\exp(1/\epsilon)]$ decoupled, related to the tunneling probability.[4] For $\epsilon=0.1$ we find

$$\bar{x}=\pm 2.4\times\left[\frac{|k|}{\lambda}\right]^{1/2},\quad W(\bar{x})=2.0780\times\left[\frac{\lambda}{|k|}\right]^{1/2},$$
$$\bar{x}=\pm 2.0\times\left[\frac{|k|}{\lambda}\right]^{1/2},\quad W(\bar{x})=0.1486\times\left[\frac{\lambda}{|k|}\right]^{1/2},$$
$$\bar{x}=\pm 1.0\times\left[\frac{|k|}{\lambda}\right]^{1/2},\quad W(\bar{x})=5.9\times 10^{-13}\times\left[\frac{\lambda}{|k|}\right]^{1/2},$$
$$\bar{x}=0,\quad W(\bar{x})=5.7\times 10^{-36}\times\left[\frac{\lambda}{|k|}\right]^{1/2}.$$

The above results show, essentially, that only the pure Gaussian configurations have a nonvanishing probability density.

By increasing ϵ, our double-Gaussian approximation to the effective potential is no longer convex downward.

At $\epsilon=1$ we obtain

$$\bar{x}=\pm 2.1710\times\left[\frac{|k|}{\lambda}\right]^{1/2}, \quad V_{\rm DG}(\bar{x})=-0.8419\times\frac{k^2}{\lambda} ,$$

$$\bar{x}=0, \quad V_{\rm DG}(\bar{x})=-0.8354\times\frac{k^2}{\lambda} ,$$

where the two absolute minima are obtained by superimposing two closely located, asymmetric Gaussians, one of which is centered near the minima of the classical potential. In this case, due to strong tunneling, one can improve upon the $\bar{x}=0$ configuration, which is always obtained by combining two symmetric Gaussians.

In our opinion, this is an interesting feature showing that in the strong-coupling case one has to enlarge the variational subspace in order to recover the convexity property of the effective potential. This can be obtained in a systematic way by taking suitable combinations of the absolute minima in which the superposition coefficients become additional variational parameters.

III. QUANTUM FIELD THEORY

Let us now consider the simple case of a self-interacting, real, scalar field governed by the Lagrangian density

$$\mathcal{L}=\tfrac{1}{2}(\partial_\mu\phi)^2-U(\phi) , \tag{3.1}$$

where $U(\phi)$ is a fourth-order polynomial in ϕ, i.e.,

$$U(\phi)=\tfrac{1}{2}m_B^2\phi^2+\frac{\lambda}{4!}\phi^4 , \tag{3.2}$$

and $\lambda\rangle 0$. The corresponding Hamiltonian density operator

$$\hat{\mathcal{H}}=\tfrac{1}{2}\hat{\pi}^2+\tfrac{1}{2}(\nabla\hat{\phi})^2+U(\hat{\phi}) \tag{3.3}$$

can be variationally evaluated within the class of normalized Gaussian wave functionals,[15]

$$\Psi_G[\phi]=(\mathrm{Det}G)^{-1/4}\exp\left[-\tfrac{1}{4}\int d^3\mathbf{x}\int d^3\mathbf{y}[\phi(\mathbf{x})-F]\times G^{-1}(\mathbf{x},\mathbf{y})[\phi(\mathbf{y})-F]\right] \tag{3.4}$$

depending on the two parameters F and Ω, respectively, associated to the field expectation value

$$\langle\Psi_G|\hat{\phi}|\Psi_G\rangle=F \tag{3.5}$$

and to the mass of the fluctuation

$$\langle\Psi_G|\hat{\phi}(\mathbf{x})\hat{\phi}(\mathbf{y})|\Psi_G\rangle=F^2+G(\mathbf{x},\mathbf{y}) , \tag{3.6}$$

with

$$G(\mathbf{x},\mathbf{y})=\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{2(\mathbf{k}^2+\Omega^2)^{1/2}} . \tag{3.7}$$

The effective potential $V_G(F)$, in the Gaussian approximation, is obtained by minimizing the energy density with respect to Ω, i.e.,

$$E(F,\Omega(F))=\int d^3\mathbf{x}\,V_G(F) , \tag{3.8}$$

with

$$E(F,\Omega)=\langle\Psi_G|\int d^3\mathbf{x}\,\hat{\mathcal{H}}|\Psi_G\rangle , \tag{3.9}$$

$\Omega(F)$ being the solution of the equation $\partial E/\partial\Omega=0$.

As shown in Ref. 4, the requirement of zero renormalized mass in the perturbative vacuum, i.e.,

$$\Omega(0)=0 , \tag{3.10}$$

implies the existence of two degenerate Gaussian minima $\pm\bar{F}$ satisfying the self-consistency equation

$$\Omega^2(\bar{F})=\frac{\lambda}{3}\bar{F}^2 , \tag{3.11}$$

and one obtains

$$V_G(\pm\bar{F})=V_G(0)-\frac{\Omega^4(\bar{F})}{128\pi^2} . \tag{3.12}$$

It is clear that the Gaussian approximation does not yield a convex effective potential and therefore one should not consider it, inside the region enclosed by the absolute minima, as a good approximation. As in the case of quantum mechanics, it is not difficult to improve on this situation

Let us denote by $\Psi_+[\phi]$ and $\Psi_-[\phi]$ the two Gaussian wave functionals corresponding, respectively, to the two absolute minima $+\bar{F}$ and $-\bar{F}$, and construct the new class of states (α and β being real numbers)

$$\tilde{\Psi}_F[\phi]=\alpha\Psi_+[\phi]+\beta\Psi_-[\phi] , \tag{3.13}$$

where the index F denotes the field expectation value

$$F=\langle\tilde{\Psi}_F|\hat{\phi}|\tilde{\Psi}_F\rangle . \tag{3.14}$$

The norm of this class of states is

$$\langle\tilde{\Psi}_F|\tilde{\Psi}_F\rangle=\alpha^2+\beta^2+2\alpha\beta\mathcal{T} , \tag{3.15}$$

with

$$\mathcal{T}=\int\{d\phi\}\Psi_+[\phi]\Psi_-[\phi] , \tag{3.16}$$

and one finds

$$\mathcal{T}=\exp\left[-\tfrac{1}{2}\bar{F}^2\int d^3\mathbf{x}\int d^3\mathbf{y}\,G^{-1}(\mathbf{x},\mathbf{y})\right] , \tag{3.17}$$

or, recalling Eq. (3.7),

$$\mathcal{T}=\exp[-\mathcal{V}\bar{F}^2\Omega(\bar{F})] , \tag{3.18}$$

$\mathcal{V}$ being the quantization volume. Therefore when $\mathcal{V}\to\infty$, $\mathcal{T}\to 0$ and each of the states [(3.13)] has the same energy as the Gaussian minima but field expectation value

$$F=(\alpha^2-\beta^2)\bar{F} \tag{3.19}$$

and now

$$\alpha^2+\beta^2=1 . \tag{3.20}$$

Therefore the energy density, evaluated within the class of states [(3.13)], is exactly flat in the region

$$-\bar{F} \leq F \leq \bar{F} \ . \tag{3.21}$$

One may wonder, in this situation, about the meaning of spontaneous symmetry breaking. Again, just like in the quantum-mechanical case, let us compute the probability of the various degenerate quantum configurations [(3.21)] enclosed by the Gaussian minima. We find

$$W(F)=|\tilde{\Psi}_F(F)|^2 \sim \left| \alpha \exp\left[-\frac{(F-\bar{F})^2 \mathcal{V}\Omega(\bar{F})}{2} \right] + \beta \exp\left[-\frac{(F+\bar{F})^2 \mathcal{V}\Omega(\bar{F})}{2} \right] \right|^2 , \tag{3.22}$$

and, when $\mathcal{V} \to \infty$, only for $F=\bar{F}$, $(\beta=0)$, or $F=-\bar{F}$, $(\alpha=0)$, the probability is not vanishing.

Similar considerations can be extended to the continuous symmetry case, as for the $O(N)$ theory considered in Ref. 16, with the obvious modification that the flat region is now enclosed by a $(N-1)$-dimensional boundary. This case, as discussed in Ref. 16, is particularly interesting since, for large N, the Gaussian potential becomes an excellent approximation to the exact effective potential (at the minima), as can be deduced from the existence of $N-1$ massless bosons (when $N \to \infty$), in agreement with the Goldstone theorem.

This concludes our brief discussion of field theory. The essential point is that a very good approximation to the exact effective potential can be easily constructed starting from the single-Gaussian approximation both in quantum mechanics, in the weak-coupling regime, and in quantum field theory.

By the way our field-theoretical analysis is restricted to translationally invariant configurations, where the total volume of the system plays an essential role in suppressing the quantum superposition. This last effect is expected to play an important role, however, when dealing with solitonlike, finite-energy classical configurations depending on a continuous parameter. Work is in progress in this direction.

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