

A variational method from the variance of energy

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Abstract. A variational method is studied based on the minimum of energy variance. The method is tested on exactly soluble problems in quantum mechanics, and is shown to be a useful tool whenever the properties of states are more relevant than the eigenvalues. In quantum field theory the method provides a consistent second-order extension to the Gaussian effective potential.

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1 Introduction

In 1873 Lord Rayleigh [1] described a variational method for calculating the frequencies of mechanical systems. Since then the Rayleigh–Ritz method has been an important tool for the approximate solution of physical problems. In quantum mechanics the method has proven very useful, and provides an upper bound for the ground-state energy, as the exact eigenstate of the Hamiltonian H yields the lowest energy expectation value.

More generally, the exact eigenstates are known to be stationary points for the expectation value of H . That is not a special property of H : for any real function f , the expectation value of the operator $f(H)$ can be proven to be stationary at the exact eigenstates of H . Thus, when the search for approximate eigenstates of H is the main issue, the expectation value of any function $f(H)$ can be used as a functional of the trial eigenstate. In general the result is different and depends on the choice of the function f unless the trial state is the exact eigenstate of H . This dependence is a measure of the accuracy of the approximate eigenstates, and can be used as a variational method of calculation whenever the description of states is more important than the determination of the corresponding energies.

In this paper the variance of H is shown to be the natural choice for a measure of the dependence on f . The resulting variational method, which we call minimal energy variance (MEV), is not novel, having been used since 1955 in numerical calculations [2]. The method has not been very popular, as the average of the square H^2 is required, and only recently have some of its interesting properties been shown in numerical quantum Monte Carlo calculations [3, 4].

We discuss in some detail the properties of MEV and show that it can be regarded as a useful complementary

tool for the properties of the eigenstates more than a substitute for the usual variational method. In that respect the MEV turns out to be of interest even for analytical calculations despite the larger amount of work required for its evaluation, which is comparable to a second-order perturbative approximation. We show that MEV is at least as general as the standard variational method, and that it can be relevant for the variational treatment of quantum field theories such as the scalar theory.

We begin by defining the MEV and discussing its general properties in Sect. 2. In fact MEV is usually described as a numerical tool in the framework of quantum Monte Carlo calculations, despite its generality. In Sect. 3 the method is illustrated by comparison of some results for exactly solvable problems in quantum mechanics (the harmonic oscillator and the hydrogen atom). In Sect. 4 MEV is shown to be relevant for the variational treatment of a scalar theory to get a consistent second-order extension of the Gaussian effective potential.

2 Definition and properties

Denoting by $|\Psi\rangle$ a generic state in the Hilbert space, the expectation value of $f(H)$ reads

$$\langle f \rangle = \frac{\langle \Psi | f(H) | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (1)$$

and the stationary condition is

$$\frac{\delta \langle f \rangle}{\delta |\Psi\rangle} = \frac{\langle \Psi | f(H) \rangle}{\langle \Psi | \Psi \rangle} - \frac{\langle \Psi | f(H) | \Psi \rangle}{\langle \Psi | \Psi \rangle^2} \langle \Psi | = 0, \quad (2)$$

which is satisfied if

$$f(H)|\Psi\rangle = \langle f \rangle |\Psi\rangle. \quad (3)$$

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The solutions of the eigenvalue problem are the stationary points of $\langle f \rangle$. Usually (with some special exceptions [5]) these solutions are the eigenstates of H . Thus, whatever f is, the stationary points of $\langle f \rangle$ yield approximate eigenstates of H . However the stationary point does depend on the choice of the function f if the generic trial state $|\Psi\rangle$ belongs to a subspace which does not contain the exact eigenstate. For instance it is well known that if the trial state $|\Psi\rangle$ is not an exact eigenstate then in general $\langle H^n \rangle \neq \langle H \rangle^n$. Thus there is no reason why the simple choice $f(H) = H$ should be the best choice. Actually any different choice for the function f would give a different weighting of the trial state in the expectation value. While the usual energy variation seems to be reasonable for the approximate evaluation of the ground-state energy, this might not be the best choice for describing the properties of the eigenstates.

We assume that the trial state $|\Psi\rangle$ is closer to the exact eigenstate when its sensitivity to f is lower. In other words, we define a distance D between the trial state and the exact eigenstate according to

$$D = \langle f(H) \rangle - f(\langle H \rangle). \quad (4)$$

Thus any choice of the function f would provide a different variational method as we know that $D = 0$ for any exact eigenstate. The most simple nontrivial choice for f is $f(H) = H^2$ and this yields the variance $\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$ as a viable candidate for the distance D .

A formal proof that the exact eigenstates of H are stationary points of σ^2 is trivial:

$$\langle \Psi | \Psi \rangle \frac{\delta \sigma^2}{\delta \langle \Psi |} = [H^2 | \Psi \rangle - \langle H^2 \rangle | \Psi \rangle] - 2 \langle H \rangle [H | \Psi \rangle - \langle H \rangle | \Psi \rangle] \quad (5)$$

and the right hand-side vanishes if $|\Psi\rangle$ is an eigenvector of H . Moreover $\sigma^2 \geq 0$ and it vanishes for any exact eigenvector, so that σ^2 has a minimum at any eigenvector (not just the ground state). In practice, whenever a trial state is close enough to an eigenstate, the variance σ^2 is expected to show a local minimum. The value of σ^2 at the minimum is a measure of the accuracy of the corresponding approximate eigenstate. Moreover the minimum of σ^2 acquires a deeper physical meaning if related to the dynamical properties of the state. The vanishing of σ for eigenstates can be seen as a consequence of the time delocalization of the stationary states. According to the Heisenberg relations $\Delta t \approx \hbar/\sigma$, a smaller energy variance allows for a longer survival of the approximate eigenstate. Thus MEV yields approximate eigenstates that best resemble the exact ones in their dynamical evolution. In that respect MEV seems to be a complementary tool for the properties of the eigenstates more than a substitute for the usual variational method, which always gives the best approximation for the eigenvalues.

3 Analytical tests

The method can be tested on exactly solvable problems: the hydrogen atom and the harmonic oscillator.

3.1 The hydrogen atom

In atomic units the Hamiltonian of the hydrogen atom is

$$H = -\frac{1}{2} \nabla^2 - \frac{1}{r}. \quad (6)$$

We choose a two-parameter trial state

$$\langle r | \Psi \rangle = N(1 - \alpha r) e^{-\beta r}. \quad (7)$$

This is the exact ground state for $\alpha = 0$, $\beta = 1$, while it is the first excited state for $\alpha = \beta = 0.5$. The expectation values of H and H^2 are easily evaluated

$$\langle H \rangle = [T_1(\alpha, \beta) - V_1(\alpha, \beta)] / [2D(\alpha, \beta)], \quad (8)$$

$$\langle H^2 \rangle = \frac{T_2(\alpha, \beta) + V_2(\alpha, \beta) - S(\alpha, \beta)}{4D(\alpha, \beta)} \quad (9)$$

where $T_1 = \beta^2(\alpha^2 - \alpha\beta + \beta^2)$, $V_1 = \beta(3\alpha^2 - 4\alpha\beta + 2\beta^2)$, $T_2 = \beta^4(3\alpha^2 + 5\alpha\beta + 5\beta^2)$, $V_2 = 4\beta^2(\alpha^2 - 2\alpha\beta + 2\beta^2)$, $S = 2\beta^3(\alpha^2 + 6\beta^2)$ and $D = (3\alpha^2 - 3\alpha\beta + \beta^2)$. The variance σ^2 has two local minima for (α, β) equal to $(0, 1)$ and $(0.5, 0.5)$, while the energy $\langle H \rangle$ only has a saddle point at $(0.5, 0.5)$. For $\alpha = \beta$ the two methods yield the same result: a minimum for $\alpha = \beta = 0.5$ where the trial state becomes the first excited state. For $\alpha = -\beta$, the trial state is quite bad: its behaviour for $r \rightarrow 0$ is

$$\langle r | \Psi \rangle \sim N(1 - \frac{1}{2}\beta^2 r^2 + \mathcal{O}(r^3)) \sim N e^{-\frac{1}{2}\beta^2 r^2}. \quad (10)$$

The variance σ^2 is quite sensitive to the shape of the wavefunction, and in this case it fails to show any minimum, while the energy $\langle H \rangle$ still has a minimum for $\beta = 1.5$. It is instructive to study the behaviour of σ^2 for a constant ratio $\alpha/\beta = k$. The trial state $|\Psi\rangle$ may get very close to an exact eigenstate if $k \approx 0$ or $k \approx 1$. In Fig. 1 the variance σ^2 is shown for several values of k . We observe a crossover from a pronounced minimum at $\beta = 0.5$ (for $k = 1$) to a pronounced minimum at $\beta = 1$ (for $k = 0$). As k becomes negative and moves away from 0, the minimum value of σ^2 raises, and eventually the minimum disappears as the trial state worsens. Conversely as k approaches 0, a minimum around $\beta = 1$ deepens until σ^2 vanishes for $k = 0$. The minimum at $\beta = 0$ is always present as in that limit the trial wavefunction becomes a constant that is an exact unbounded eigenstate with a vanishing energy. Thus at variance with the standard variational method, MEV may be used for approximating excited states without having to insert orthogonality conditions: a local minimum appears whenever the trial state is close enough to an exact eigenstate. Moreover the sensitivity of σ^2 discards bad approximations as the minimum disappears for the worse trial states. Whenever a minimum is present its value is by itself a measure of the accuracy of the state as $\sigma^2 = 0$ for the exact eigenstate.

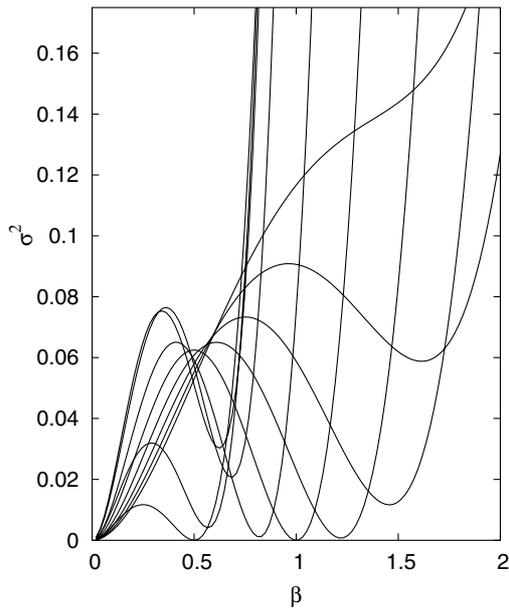


Fig. 1. The variance σ^2 for approximate eigenstates of the hydrogen atom. The trial wavefunction is defined according to (7) with $\alpha = k\beta$ and $k = 1.0, 0.8, 0.6, 0.4, 0.2, 0.0, -0.2, -0.4, -0.6, -0.8$. The minimum moves from left to right when k decreases, and disappears at $k \approx -0.7$

3.2 The harmonic oscillator

Other insights on the method come from the study of the simple harmonic oscillator. Let us consider the Hamiltonian

$$H = \frac{p^2}{2} + \frac{1}{2}\omega_0^2 x^2 \tag{11}$$

which describes an oscillator whose frequency is ω_0 . Let us denote by $|n, \omega_0\rangle$ the exact eigenstates with energies $E_n = \hbar\omega_0(n + 1/2)$. As a trial state we may take a linear combination of the lower-energy eigenstates of a generic oscillator whose frequency is ω :

$$|\Psi\rangle = |0, \omega\rangle + \alpha|1, \omega\rangle \tag{12}$$

where both α and ω are variational parameters. The trial state is the exact ground state of H for $\alpha = 0$ and $\omega = \omega_0$, while it gives the first excited state for $\alpha \rightarrow \infty$ and $\omega = \omega_0$. The calculation of the expectation values of H and H^2 is trivial: in units of $\hbar\omega_0/2$ we may express them as

$$\langle H \rangle = \cosh(\ln x) f_3(\alpha), \tag{13}$$

$$\langle H^2 \rangle = 3 \sinh^2(\ln x) f_5(\alpha) + f_9(\alpha) \tag{14}$$

where $x = \omega_0/\omega$ and $f_n(\alpha) = (1 + n\alpha^2)/(1 + \alpha^2)$ is a smooth increasing function of α ranging from 1 (at $\alpha = 0$) to n (for $\alpha \rightarrow \infty$).

The variance follows as

$$\sigma^2 = \frac{1}{\cosh^2(\ln \alpha)} + g(\alpha) \sinh^2(\ln x) \tag{15}$$

where $g(\alpha) = 2(3\alpha^4 + 6\alpha^2 + 1)/(1 + \alpha^2)^2$ is a smooth increasing function of α ranging from 2 (at $\alpha = 0$) to 6 (for $\alpha \rightarrow \infty$).

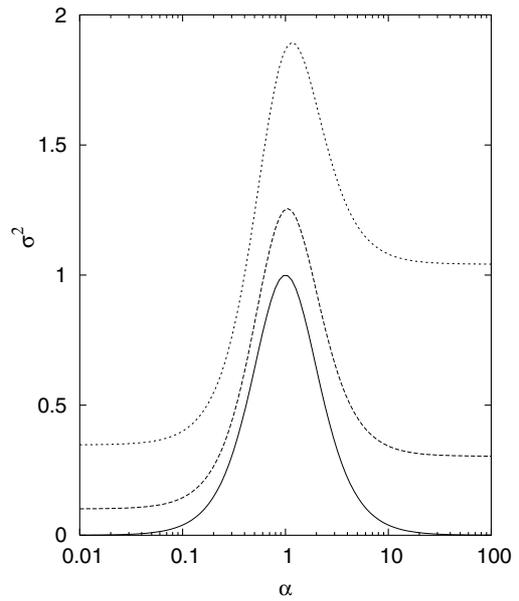


Fig. 2. The variance σ^2 for approximate eigenstates of the harmonic oscillator. The trial state is defined according to (12) with α ranging from $\alpha = 0$ (ground state) to $\alpha \rightarrow \infty$ (first excited state) while $\omega_0/\omega = x$ is taken to be $x = 1$ (lower curve), $x = 1.25$ and $x = 1.5$ (upper curve). Approaching the exact eigenstates ($x \rightarrow 1$) the minima decrease and eventually vanish

First of all we mention that both methods must predict the exact values of α even for $x \neq 1$ (i.e. $\omega \neq \omega_0$): in fact at any ω the states $|0, \omega\rangle$ and $|1, \omega\rangle$ have different symmetry properties, and thus the trial state can be an eigenstate of parity only for $\alpha = 0$ (even) or $\alpha \rightarrow \infty$ (odd). Actually we may observe that $\alpha = 0$ and $\alpha \rightarrow \infty$ are stationary points of $\langle H \rangle$ and σ^2 for any choice of the parameter x . This is evident for $\langle H \rangle$ as in (13) the contributions of α and x are in different factors. We always get a minimum for $\alpha = 0$ (ground state), while the limit $\alpha \rightarrow \infty$ is a maximum (first excited state). Whatever α is, $\langle H \rangle$ has a unique stationary point for $x = 1$ where the hyperbolic cosine has a minimum. From (15) we see that the variance follows the same path: for any choice of α a minimum occurs at $x = 1$ where the hyperbolic sine vanishes. If we set $x \neq 1$, then we can explore the dependence of the variance on α . As we move from $x = 1$ (i.e. $\omega = \omega_0$), the trial state worsens. We still find two minima at $\alpha = 0$ and $\alpha \rightarrow \infty$, but the minimum value of the variance increases as the state gets worse. In Fig. 2 the variance is shown for some values of x . From (15) we see that, at the minima, $\sigma^2 = g(\alpha) \sinh^2(\ln x)$ so that we get a larger variance $\sigma^2 = 6 \sinh^2(\ln x)$ at the first excited state ($\alpha \rightarrow \infty$), and a smaller variance $\sigma^2 = 2 \sinh^2(\ln x)$ at the ground state ($\alpha = 0$). Thus the trial state is a better approximation for the ground state than it is for the first excited state.

4 Scalar theory

In quantum field theory the properties of vacuum are more relevant than its energy, which is not finite anyway. For

instance the symmetry-breaking mechanism and the mass of the Higgs boson depend on the structure of the true vacuum. Thus we argue that the use of MEV could give rise to new insights into the ground-state properties of relevant field theories such as the scalar theory. In fact we show that MEV may be used for improving the Gaussian effective potential (GEP), a useful variational tool which has been discussed by several authors since 1974 [6–13]. The GEP has many merits, and has been successfully applied to physical problems ranging from electro-weak symmetry breaking [14] and scalar theories [13], to superconductivity in bulk materials [15] and films [16]. A second-order extension of the Gaussian approximation would be desirable for a better understanding of the symmetry-breaking transition. In fact the GEP is sometimes known to predict a first-order transition even when the phase change should be continuous. Moreover, the GEP fails to show a minimum for some ranges of parameters. Attempts to improve the GEP have not been so successful: the post-Gaussian effective potential (PGE) discussed by Stancu and Stevenson [17] fails to reach a minimum for any finite value of the variational parameter, which is fixed by the vanishing of the second derivative [18]. A way out has been studied by Tedesco and Cea [19], who take the variational parameter fixed at the first-order value. In this paper we point out that the minimum of variance would be a viable tool for determining the variational parameter, and we show that this choice allows a useful second-order extension of the GEP.

The GEP can be seen as an improved first-order perturbative approximation. Let us decompose the Hamiltonian into two parts as $H = H_\Omega + V_\Omega$, where H_Ω is any solvable Hamiltonian that depends on the parameter Ω , while $V_\Omega = H - H_\Omega$. The decomposition itself depends on the parameter Ω . The ground state of H_Ω satisfies the eigenvalue equation

$$H_\Omega|\Psi_\Omega\rangle = E_\Omega|\Psi_\Omega\rangle. \quad (16)$$

Then the first-order perturbative approximation for the lower eigenvalue of H follows

$$E = E_\Omega + \langle\Psi_\Omega|V_\Omega|\Psi_\Omega\rangle. \quad (17)$$

The minimum of E can be found by a variation of the parameter Ω , and at the minimum point $\Omega = \Omega_0$ we get the best decomposition of H (in the sense that the first-order perturbative approximation yields the lower energy). However E is the expectation value of the full Hamiltonian H , and the method is a genuine variational method: the trial state is the eigenstate $|\Psi_\Omega\rangle$, which depends on the parameter Ω according to (16). In the GEP H_Ω is the Hamiltonian of a free scalar field whose mass is Ω , and its ground state $|\Psi_\Omega\rangle$ is a Gaussian functional of fields.

The PGE [17] is equivalent to the second-order perturbative evaluation of the vacuum ground-state energy (effective potential). It arises from the sum of all the second-order connected one-particle irreducible diagrams without external legs. It can be proven to be equivalent to the cumulant expansion discussed by Kleinert [20], and then the second-order correction $\delta E^{(2)}$ is basically equivalent to the

variance up to a sign

$$\delta E^{(2)} = \langle V_\Omega \rangle^2 - \langle V_\Omega^2 \rangle = \langle H \rangle^2 - \langle H^2 \rangle = -\sigma^2. \quad (18)$$

Thus the minimum of the variance is equivalent to the minimum absolute value of the second-order correction. According to the asymptotic convergence of the perturbative expansion we know that a minimum of the second-order correction is equivalent to a minimum of the error that we expect in the first-order expansion. From this point of view the minimum of the variance singles out the best perturbative expansion.

The explicit expression for the second-order effective potential $V^{(2)}$ has been reported in [17] as a function of the vacuum expectation value of the field $\langle\phi\rangle = \varphi$ for a scalar theory whose action reads

$$S[\phi] = \int d^d x \left[\frac{1}{2} \phi(x) (-\partial^2 + m^2) \phi(x) + \lambda \phi^4(x) \right] \quad (19)$$

in a d -dimensional Euclidean space. The second-order effective potential is given by

$$V^{(2)} = V^{(1)} + \delta E^{(2)} \quad (20)$$

where $V^{(1)}$ is the first-order GEP

$$V^{(1)} = I_1(\Omega) + \frac{1}{2} m^2 \varphi^2 + \lambda \varphi^4 + \frac{1}{2} I_0(\Omega) [m^2 - \Omega^2 + 12\lambda\varphi^2 + 6\lambda I_0(\Omega)] \quad (21)$$

and the second-order correction reads

$$\delta E^{(2)} = - \left\{ \frac{1}{8} I^{(2)}(\Omega) [m^2 - \Omega^2 + 12\lambda\varphi^2 + 12\lambda I_0(\Omega)]^2 + 8\lambda^2 \varphi^2 I^{(3)}(\Omega) + \frac{1}{2} \lambda^2 I^{(4)}(\Omega) \right\}. \quad (22)$$

Here $I^{(n)}(\Omega)$ and $I_n(\Omega)$ are the integrals defined according to [17]

$$I_1(\Omega) = \frac{1}{2} \int \frac{d^d p}{(2\pi)^d} \ln(p^2 + \Omega^2), \quad (23)$$

$$I_0(\Omega) = \int \frac{d^d p}{(2\pi)^d} \frac{1}{p^2 + \Omega^2}, \quad (24)$$

$$I^{(n)}(\Omega) = n! \int d^d x [G(x)]^n \quad (25)$$

where $G(x)$ is the free-particle Green function

$$G(x) = \int \frac{d^d p}{(2\pi)^d} \frac{e^{ipx}}{(p^2 + \Omega^2)}. \quad (26)$$

Most of these integrals are diverging and must be regularized. The search for the minimum of $V^{(2)}$ yields a gap equation for the free field mass Ω . A numerical analysis of this gap equation shows that there is no minimum for the second-order effective potential, while the second-order

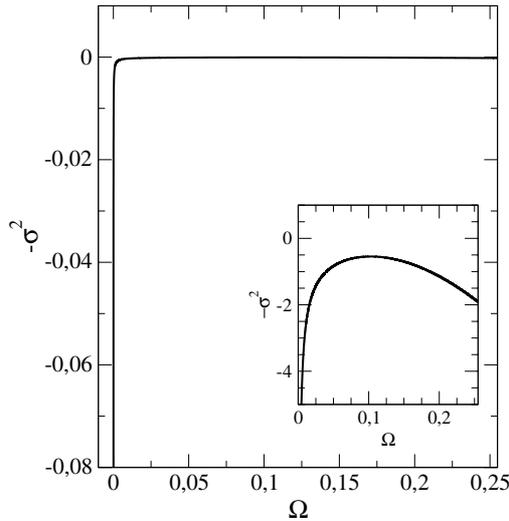


Fig. 3. The second-order correction (the variance, up to a sign) for the effective potential in $\lambda\Phi^4$ scalar theory. The values for the parameters are: $d = 3$, $m^2/\Lambda^2 = -0.06$ and $\lambda/\Lambda = 0.1$, $\varphi/\sqrt{\Lambda} = 0.1$. Note that it is unbounded, so that the total effective potential cannot have a minimum whatever value the variational parameter Ω takes; as shown in the inset graph (an enlargement with σ^2 unit scaled by a factor 10^4), however, it has, by itself, a pronounced maximum, making MEV a reasonable alternative to PGEP, where the vanishing of the second derivative of $V^{(2)}$ is required

correction by itself (the variance) has a pronounced minimum for a broad range of the parameters.

The second-order correction has been evaluated as a function of the bare parameters m and λ , and the variational parameter Ω . An energy cutoff Λ has been inserted to regularize all the diverging integrals. In Fig. 3 $\delta E^{(2)}$ versus Ω is reported, for $d = 3$ and for the set of parameters $m^2/\Lambda^2 = -0.06$, $\lambda/\Lambda = 0.1$, $\varphi/\sqrt{\Lambda} = 0.1$. According to (18) it turns out to be negative; moreover, as is clear from the figure, the second-order correction, while having a maximum when its absolute value is minimum (which is the minimum of the variance: see the inset in Fig. 3), is not bounded: this explains why the total effective potential fails to reach a minimum for any choice of the free mass Ω .

The minimum of σ^2 yields a best value $\Omega = \Omega_0$ for each value of the shift φ . Insertion in $V^{(2)}$ gives our second-order effective potential. This should be compared to the PGEP of [17] where the best Ω is obtained by the vanishing of the second derivative of $V^{(2)}$ [18].

In Fig. 4 our second-order effective potential is reported (the same $d = 3$ and bare parameter values as those in Fig. 3 were used). For this set the system is close to its transition point. For comparison in the same figure we also show the standard first-order GEP, and the PGEP evaluated according to [17]. For $d = 3$ the system may be regarded as a static statistical model for a phase transition in three-dimensional space (Ginzburg–Landau action). The predictions of this model can be tested by comparison with the experimental data on the phase transition of different systems like superfluids and superconductors. Unfortunately the simple GEP predicts a first-order transition in this case (while

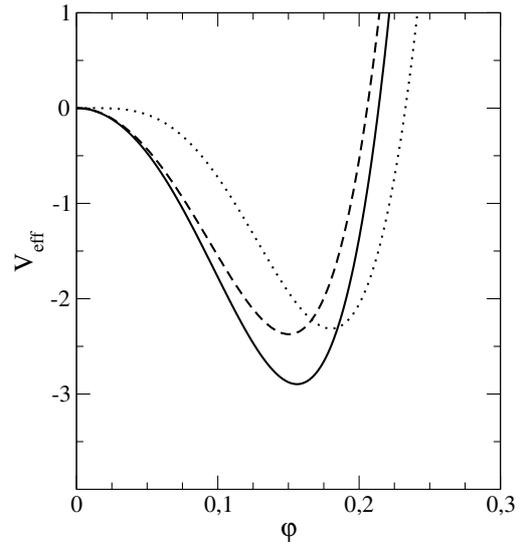


Fig. 4. The second-order effective potential evaluated by the method of minimum variance (solid line) for $d = 3$, $m^2/\Lambda^2 = -0.06$ and $\lambda/\Lambda = 0.1$. For comparison the PGEP (dashed line) and the simple first-order GEP (dotted line) are reported. The effective potential is scaled by a factor 10^5 , while the field shift φ is in units of $\sqrt{\Lambda}$

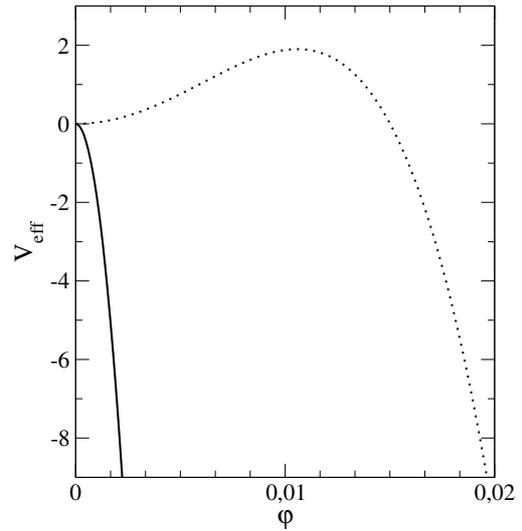


Fig. 5. An enlargement (the effective potential is scaled by a factor 10^9) of the $\varphi = 0$ region in Fig. 4; the GEP (dotted line) predicts a first-order transition with the point at $\varphi = 0$ being a local minimum; instead, the MEV (solid line) predicts a continuous transition (as it should be for superconductivity), thus providing a consistent variational second-order extension of the GEP

the transition is known to be continuous). In Fig. 5 an enlargement of the $\varphi = 0$ area makes these reasonings more evident: the GEP (dotted line) is an increasing function up to a maximum (the point $\varphi = 0$ is a local minimum). Actually the phase transition occurs when the true minimum rises more than the local minimum (first-order transition). Our second-order potential (solid line), evaluated by MEV, predicts a continuous transition (as it should be), with the point at $\varphi = 0$ *always* being a local maximum in the broken

phase. Thus the method provides a consistent second-order extension of the GEP while retaining its variational character.

We conclude that, while MEV has been shown recently to be a useful tool in numerical quantum Monte Carlo calculations, its potential has not yet been fully explored. Whenever the properties of states are more relevant than the eigenvalues, MEV provides a viable variational method which can be used in analytical and field-theory calculations as a complementary tool.

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