The Principle of Stationary Variance in Quantum Field Theory

Fabio Siringo

Dipartimento di Fisica e Astronomia dell’Università di Catania, INFN Sezione di Catania, Via S.Sofia 64, I-95123 Catania, Italy
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The principle of stationary variance is advocated as a viable variational approach to quantum field theory. The method is based on the principle that the variance of energy should be at its minimum when the state of a quantum system reaches its best approximation for an eigenstate. While not too much popular in quantum mechanics, the method is shown to be valuable in quantum field theory, and three special examples are given in very different areas ranging from Heisenberg model of antiferromagnetism to quantum electrodynamics and gauge theories.

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Since when Lord Rayleigh described his method for calculating the frequencies of a mechanical system in 1873[1], the variational method has become very popular. In quantum mechanics (QM), the variational method follows from the well known property that the expectation value of the Hamiltonian is stationary when the quantum state is an eigenstate. However, that property is shared with any function of the Hamiltonian, and a more general variational method can be introduced by looking for the stationary points of other functions of the Hamiltonian[2,3]. Among them, the variance has the important physical features of being positive, bounded from below, and vanishing at the exact eigenstates. Moreover, by Heisenberg relations, its finite value gives a measure of the life-time of an approximate eigenstate.

While the principle of stationary variance is not very popular in QM, it can be very useful in quantum field theory (QFT). In this letter we show that in QFT the search for the stationary points of the variance provides a viable variational approach to selected problems where the standard variational method is known to fail or give trivial results. Should a strong coupling preclude the use of perturbation theory, the stationary variance would be a valid alternative to numerical lattice simulations. We give three examples of well known extended physical systems where the standard variational method fails to produce an acceptable description, while the principle of stationary variance provides reasonable nontrivial results: the Heisenberg limit of the half-filled Hubbard model of antiferromagnetism, the simple theory of a self-interacting scalar field, and quantum electrodynamics (QED).

In QM, denoting by $\langle \psi \rangle$ the expectation value of the operator $O$ in the state $|\psi\rangle$, the variance of the Hamiltonian $H$ can be written as $\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$ and satisfies

$$\langle \psi | \frac{\delta \sigma^2}{\delta |\psi\rangle} | \psi \rangle = (\langle H^2 \rangle - \langle H \rangle^2) |\psi\rangle - 2\langle H \rangle (\langle H \rangle |\psi\rangle) |\psi\rangle.$$  \hfill (1)

Thus the first variation of $\sigma^2$ is zero if the state $|\psi\rangle$ is an eigenstate of $H$. Since $\sigma^2 \geq 0$ in any state, and $\sigma^2 = 0$ in eigenstates, whenever a trial state approaches an eigenstate the variance is expected to be stationary and to show a local minimum. Of course that happens for any eigenstate, not just the ground state, and some caution is required when the trial state can approach different eigenstates. In Ref.[2] a detailed discussion of the method is reported for simple problems of QM. For instance in the simple case of an hydrogen atom, and a trial state

$$\langle r |\psi \rangle = (1 - \eta br)e^{-br}$$  \hfill (2)

that, in atomic units, is the exact ground state for $\eta = 0$, $b = 1$ and the first excited state for $\eta = 1$, $b = 0.5$, the variance is reported in Fig.1 as a function of $b$ for several values of $\eta$. We observe a pronounced minimum when the trial state approaches one of the eigenstates.
In QM, the predictive power of the standard variational method can be improved by just increasing the number of free parameters, thus enlarging the subspace spanned by the trial wave function. There is no real utility in a more complex second order calculation, like that of variance, that would require the matrix elements of the square of $H$. In QFT, because of calculability, the trial functional must be Gaussian, the standard variational method leads to the Gaussian effective potential (GEP) \[11\] and there is no obvious way to improve the approximation. In fact, several extended physical systems are described by field theories that are not suited to be described by a first order approximation like the GEP. Second order terms might give important contributions that could be captured by a second order variational method like that of stationary variance.

As a first example, let us consider the half-filled two-dimensional Hubbard model of a narrow band conductor with a strong on-site repulsive correlation\[20\].

\[
H = -t \sum_{<ij>,\alpha} C_{i\alpha}^\dagger C_{j\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]  

(3)

where $C_{i\alpha}^\dagger$ ($C_{i\alpha}$) are creation (annihilation) operators for the electrons, $\alpha = \pm$ is the spin projection, $n_{i\alpha} = C_{i\alpha}^\dagger C_{i\alpha}$ are number operators and the site indices $i, j$ run over first neighbors on a square lattice. The Fermi liquid is known to be unstable towards an antiferromagnetic (AF) ground state\[20\]. If $U$ is large, we can take the simultaneous eigenstates of the number operators as a basis set, and each of these states can be labeled by a string of charges $n_{i\alpha} = 0, 1$, with $\sum_{i\alpha} n_{i\alpha} = N$ where $N$ is the total number of electrons that is assumed to be equal to the number of lattice sites. For $t = 0$ there is a massive degeneracy in the system: the ground state has an energy $E = 0$ and is given by any linear combination of the degenerate $2^N$ states $|m\rangle_0$ with no double occupancy and a single electron on each site (with $n_{i\uparrow} + n_{i\downarrow} = 1$); the first excited state has $E = U$ and is given by the degenerate states $|m\rangle_1$ with a single double occupancy (and a single hole), etc. We expect that the degeneracy would be removed by a small but finite hopping term $t \ll U$. In this strong coupling limit, the hopping term could be regarded as a small perturbation. It is quite obvious that first order perturbation theory and standard variational method are useless in the present case: if we define by $H_0 = H_{t=0}$ the correlation term, and by $V_t = H_{U=0}$ the hopping term, so that $H = H_0 + V_t$, even for $t \neq 0$ we always find

\[
\langle m'|V_t|m\rangle_0 = 0
\]  

(4)

and then $\langle \Psi|H|\Psi\rangle = 0$. The excited states cannot be neglected even when they are very far at $E = U$, so that we need the second order perturbative correction or a second order variational method if we want to keep the trial state $|\Psi\rangle$ in the ground state subspace. In fact the failure of the first order approximations is due to the vanishing of all first order matrix elements in the ground state subspace according to Eq. (3).

Let us look at the variance: since $\langle \Psi|H|\Psi\rangle = 0$, the variance can be written as

\[
\sigma^2 = \langle \Psi|H^2|\Psi\rangle = \sum_m \langle \Psi|V_t|m\rangle_1 \cdot \langle m|V_t|\Psi\rangle
\]  

(5)

where the sum runs over first excited states only, and $\langle 1|m|0\rangle^2 = t^2$ when the states differ for the hopping of a single electron between first neighbor sites or vanishes otherwise. In fact, these matrix elements allow for some electron motion among first neighbors, and the matrix elements of the variance $\sigma^2(m|H^2|m')_0$ differ from zero in the ground state subspace, if the states $m \neq m'$ differ by a spin flip of two first neighbor electrons. Actually, because of Pauli principle, the matrix elements of $H^2$ enumerate all the first neighbor pairs of electrons with opposite spin that can hop and go back from one site to the other by the second order process. By a straightforward calculation, in the single occupancy subspace, $H^2$ can be written up to a constant as an effective Hamiltonian in terms of local spin operators $\vec{S}_i$

\[
H^2 = -2t^2 \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j = -UH_H
\]  

(6)

where $H_H$ is the well known Heisenberg Hamiltonian of the spin system. We conclude that, in the single occupancy subspace spanned by $|\Psi\rangle$, the eigenstates of the variance are the eigenstates of the Heisenberg Hamiltonian that is known to be the exact strong coupling limit of the Hubbard model at half-filling, and has an AF ground state. Thus, in the same subspace, the stationary states of the variance must be the eigenstates of the Heisenberg model, and the principle of the stationary variance yields the correct AF ground state of the system. This simple example tells us that the same method of the stationary variance could be useful for gauge theories where the minimal coupling does not give any contribution to the effective potential in first order approximations like the GEP. We need a Lagrangian version of the method that has been developed for the simple theory of a self-interacting scalar field.\[2\] [3].

Actually, even for the simple scalar theory, the standard variational description by the GEP presents some shortcomings that can only be cured by a second order approximation. For instance the order of the transition that is known to be second order, but is weakly first order in the GEP.\[3\]. The problem is solved by inclusion of second order terms in a post Gaussian effective potential (PGEP)\[21\], but the second order effective potential is not bounded from below, and has no stationary points. On the other hand the method of stationary variance
is perfectly viable, and yields a second order variational approximation that improves the GEP and predicts a second order transition\[2\]. Thus the scalar theory is the best example for illustrating the Lagrangian approach to the method. The Lagrangian reads
\[ \mathcal{L} = \frac{1}{2} \partial^\mu \phi \partial_\mu \phi - \frac{1}{2} m^2 \phi^2 - \lambda \phi^4. \] (7)

We define a shifted field \( \phi = \phi - \varphi \) where \( \varphi \) is a constant background, and split the action functional as \( S[\phi] = S_0[h] + S_I[h] \) where \( S_0[h] \) is an arbitrary trial Gaussian functional, quadratic in the fields, that can be thought as the action of a free particle theory. It can be written as
\[ S_0[h] = \frac{1}{2} \int h(x) g^{-1}(x,y) h(y) d^4 x d^4 y \] (8)
where \( g(x,y) \) is an unknown trial propagator. One of the main merits of the Lagrangian approach is that the effective action \( \Gamma[\varphi] \) can be evaluated as a sum of Feynman diagrams by the general representation\[22\]
\[ e^{\Gamma[\varphi]} = \int_{1PI} D_h e^{i S[\varphi + h]} = \int_{1PI} D_h e^{i S_0[h]} e^{i S_I[h]} \] (9)
equivalent to the sum of all the one-particle-irreducible (1PI) vacuum diagrams for the action functional \( S[\varphi + h] \), with \( S_I \) that plays the role of the interaction. In terms of the quantum average
\[ \langle \phi \rangle = \frac{\int_{1PI} D_h e^{i S_0[h]} \phi}{\int_{1PI} D_h e^{i S_0[h]}}, \] (10)
the effective action can be written as an expansion in moments of \( S_I \)
\[ i \Gamma_n[\varphi] = \sum_{n=0}^{\infty} i \Gamma_n[\varphi] = i \Gamma_0 + \langle i S_I \rangle + \frac{1}{2!} \left( \langle i S_I \rangle^2 \right) + \frac{1}{3!} \left( \langle i S_I \rangle^3 \right) + \ldots \] (11)
that is the sum of all connected 1PI vacuum diagrams, while \( \Gamma_0 \) follows exactly from the quadratic \( S_0 \). Thus we can use perturbation theory for evaluating the effective potential \( V[\varphi] = -\Gamma[\varphi]/\Omega \) where \( \Omega \) is the total spacetime volume. On the other hand, since the exact action does not depend on the arbitrary choice of \( S_0 \) (and \( S_I \)), we can optimize the splitting of \( S \) by a variational criterion that makes the effects of the interaction \( S_I \) smaller in the vacuum of \( S_0 \), yielding a convergent expansion even without any small parameter\[22\]. The principle of stationary variance suggests itself, since by Eq.(11) we see that the second order term of the effective potential is \( V_2 = -\sigma_J^2/2\Omega \) where \( \sigma_J \) is the variance of the Euclidean form of \( S_I \), as follows immediately by Wick rotating. The variance would be zero if the vacuum of \( S_0 \) were an exact eigenstate of \( S_I \), while a minimal variance is expected to optimize the convergence of the expansion. It is quite obvious that \( \sigma_J \) is equal to the variance of the total action \( S \), because powers of \( S_0 \) only give disconnected contributions. Thus in this approach the variance of the Lagrangian is used instead of the variance of the Hamiltonian. The free parameters can be fixed by a stationary condition for the second order term of the effective potential \( V_2 \), yielding a second order variational criterion. In fact, while the variance is bounded and \( \sigma_J^2 > 0 \), the second order effective potential is not, as the minimum of \( V_2 \) would be a maximum for \( \sigma_J^2 \). Actually, by insertion of a free particle trial propagator \( g^{-1}(k) = k^2 - M^2 \) the stationary (minimum) point of \( \sigma_J \) yields a solution for the mass \( M \), and the corresponding second order potential shows a continuous phase transition improving on the simple first order GEP\[2\]. However, the approximation can be improved further by considering any functional form for \( g^{-1}(k) \), and imposing the stationary condition by the functional condition \( \delta V_2/\delta g = 0 \) that becomes an integral equation for the optimal propagator \( g \). Moreover, there is no need to evaluate the effective potential as the stationary condition can be derived by the self-energy directly, making use of the general connection
\[ \frac{\delta V_n}{\delta g(k) = \frac{i}{2} \left( \Sigma_n(k) - \Sigma_{n-1}(k) \right) \] (12)
where \( \Sigma_n \) is the nth-order self-energy term. This connection follows by Wick’s theorem, and a detailed derivation will be published elsewhere\[3\]. Taking \( n = 2 \), the integral equation for the trial propagator \( g \) can be simply written as \( \Sigma_2 = \Sigma_1 \).

This machinery seems to be suited for theories with gauge interacting fermions, since the minimal coupling has no effect on the first order potential, and other variational approaches like GEP and PGE give trivial results\[24\]. That is a circumstance that we already encountered in the Heisenberg limit of the Hubbard model. Let us consider the simple case of QED with a single massive fermion
\[ \mathcal{L} = \bar{\Psi}(i\partial - eA - m)\Psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2} (\partial_\mu A^\mu)^2 \] (13)
where the last term is the gauge fixing term in Feynman gauge, and \( F_{\mu\nu} \) is the electromagnetic tensor. We must introduce two trial propagators in \( S_0 \), one \( D_{\mu\nu}(k) \) for photons, and the other \( G^{\mu\nu}(k) \) for fermions. These are unknown trial functions, and in general differ from the bare propagators \( \Delta_{\mu\nu}^{-1}(k) = -\eta_{\mu\nu} k^2 \), \( g_{\mu\nu}^{-1}(k) = k - m \).

The stationary conditions for the effective potential can be derived by the general connection to self-energy and polarization functions
\[ \frac{\delta V_n}{\delta G^{\mu\nu}(k) = -i \left( \Sigma_n^{ba}(k) - \Sigma_{n-1}^{ba}(k) \right)} \] (14)
\[ \frac{\delta V_n}{\delta D_{\mu\nu}(k) = \frac{i}{2} \left( \Pi^{\mu\nu}_n(k) - \Pi^{\mu\nu}_{n-1}(k) \right)} \] (15)
These equations generalize Eq. [12], and their detailed derivation will be given in Ref. [3]. The criterion of
stationary variance is enforced by imposing that $δV_2/δG = 0$
and $δV_2/δD = 0$, that according to Eqs. [14], [15] are equivalent to $Σ_2 = Σ_1$ and $Π_2 = Π_1$. Self-energy and
polarization functions follow by use of the standard perturbation theory with an optimized interaction $S_I = S - S_0$,
as for the scalar theory. While the standard variational method gives the trivial result $D = Δ, G = g_m$, the stationary equations for the variance can be written as

$$G(k) = g_m(k) - g_m(k) · Σ^*_{2}(k) · g_m(k)$$

$$D_{μν}(k) = Δ_{μν}(k) - Δ_{μλ}(k) · Π^*_{2λ}(k) · Δ_{νλ}(k)$$

(16)

where $Π^*_{2}, Σ^*_{2}$ are the usual proper two-point functions

$$Σ^*_{2}(k) = ie^2 ∫ \frac{d^4p}{(2\pi)^4} \gamma^μ G(k + p)γ^ν D_{μν}(p)$$

$$Π^*_{2μν}(k) = -ie^2 ∫ \frac{d^4p}{(2\pi)^4} Tr \{G(p + k)γ^μG(p)γ^ν\}.$$  (17)

Of course these one-loop terms contain divergences, and a regularization scheme must be adopted. That is not a diffi-
cult task, as in the present Lagrangian approach we can use the standard techniques of perturbation theory [21],
and renormalize bare parameters and functions order by order. A detailed description of renormalization by di-

dimensional regularization will be given in Ref. [25].

The stationary equations Eqs. [10] are a set of coupled integral equations, and their numerical solution would be equivalent to the sum of an infinite set of Feynman graphs. They are expected to hold even in the limit of
strong coupling, as they derive from a variational crite-

rion, and lead to nontrivial physical insights. While a

strong coupling limit of QED is not of any

real phenomenological interest, the stationary variance could be an important tool for a non-perturbative an-

alytical study of non-Abelian gauge theories and QCD,

wherever the large strength of the interaction does not al-

low the use of perturbation theory. Since we have shown

that the principle of stationary variance provides reason-

able results in very different areas of physics, we expect

that its extension to non-Abelian gauge theories might be

very useful for a better understanding of the low energy phenomenology of strong interactions.

$$G \approx g_m, D \approx Δ,$

and substituting back in the proper self energy $Σ^*_{2}$, then Eq. [19] would become exactly equal to the one-loop propagator of QED. Thus we conclude

that in the weak coupling limit the principle of sta-

tionary variance reproduces the standard results of QED.

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