A novel variational approach for Quantum Field Theory: example of study of the ground state and phase transition in Nonlinear Sigma Model

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We discuss a novel form of the variational approach in Quantum Field Theory in which the trial quantum configuration is represented directly in terms of relevant expectation values rather than, e.g., increasingly complicated structure from Fock space. The quantum algebra imposes constraints on such expectation values so that the variational problem is formulated here as an optimization under constraints. As an example of application of such approach we consider the study of ground state and critical properties in a variant of nonlinear sigma model.

The variational approach is one of the corner-stones of nonperturbative methods in Quantum Mechanics and Quantum Field Theory. In this approach, the expectation value of the Hamiltonian is analyzed on a set of quantum configurations of specific form and its minimum is sought. Variational Method takes roots in Ritz Theorem [1] which states that for a hermitian Hamiltonian operator with the spectrum bounded from below

$$\langle H\rangle = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} \geq E_0, \tag{1}$$

for any quantum state Φ. Here E_0 is the lowest eigenvalue of H. Ritz theorem can be transparently motivated using the fact that hermitian operator should have a complete set of eigenstates, i.e. an arbitrary quantum state can be represented as a linear superposition of the Hamiltonian eigenstates. Then, after doing a simple algebra one can get

$$\langle\Phi|H|\Phi\rangle = \sum_{n,n'} \phi_n^* \phi_{n'} \langle\psi_n|H|\psi_{n'}\rangle = \sum_n |\phi_n|^2 E_n \langle\psi_n|\psi_n\rangle \geq E_0 \langle\Phi|\Phi\rangle. \tag{2}$$

Here $|\Phi\rangle = \sum_n \phi_n|\psi_n\rangle$ and $|\psi_n\rangle$ are eigenstates of Hamiltonian H with eigenvalues $E_n \geq E_0$. From this simple argument, it follows that one will get an upper limit for the ground state energy if one computes the Hamiltonian expectation value on arbitrary quantum state Φ. This suggests a way to generate a useful estimate for the ground state energy by considering a class of trial quantum states $\{\Phi_\alpha, \alpha \in \mathbf{A}\}$ and minimizing $E(\alpha) = \frac{\langle\Phi_\alpha|H|\Phi_\alpha\rangle}{\langle\Phi_\alpha|\Phi_\alpha\rangle}$ with respect to parameter α.

The variational approach found a wide range of applications due to its simplicity, possibility of analytical results and important nonperturbative content. One of the simplest examples is the problem of Hydrogen-like atom which is described in dimensionless unitsby the Hamiltonian

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}. \tag{3}$$

Choosing an exponential trial wavefunction $\Phi_\alpha(r) = e^{-\alpha r}$, one trivially obtains

$$\langle H \rangle = \frac{1}{2}\alpha(\alpha - 2) \tag{4}$$

from which the solution $\alpha = 1$, $E = -0.5$ immediately follows. In this case, the variational estimate is in fact the exact answer.

Many examples of the original applications of variational method in Quantum Mechanics for computation of the energy levels of simple molecules can be found in the literature. In the later time, variational method had been employed increasingly for the precision many-body calculations of the ground state energies and first excited levels of atoms and simple molecules. In theoretical studies, variational method is often used to derive important nonperturbative constraints, e.g. asymptotic properties, on quantum-mechanical models. First work using variational method in Quantum Field Theory dates back to 1960th since it had been applied to a variety of atomic, nuclear and quark problems. In QFT, variational method is commonly used to investigate stability of the vacuum as well as to study dynamics of one- or two-particle excitations [2]. Also, the conclusion about possibility of color-superconductivity in QCD vacuum can be justified by considering the trial states with quark-quark vacuum condensations. The use of variational principle to formulate nonperturbative equations of state for few-body systems had also enjoyed growing popularity [3,4].

In QFT, the variational principle is derived from the equation for the covariant mass

$$P^\mu P_\mu |\Phi\rangle = M^2 |\Phi\rangle, \tag{5}$$

where P^μ is the momentum-energy operator. In the Center of Momentum Frame, $\vec{P}|\Phi\rangle = 0$, this becomes

$$\begin{aligned} (P^0)^2|\Phi\rangle &= M^2|\Phi\rangle, \\ P^0|\Phi\rangle &= \pm M|\Phi\rangle. \end{aligned} \tag{6}$$

Eq.(6) describes two energy spectra identical up to the change of sign which are conventionally associated with particle and antiparticle sectors of a field-theoretical model. By excluding spectrum of negative energies, one arrives at

$$\frac{\langle \Phi | P^0 | \Phi \rangle}{\langle \Phi | \Phi \rangle} = E[\Phi] \geq E_0 \tag{7}$$

or, equivalently,

$$\langle \delta\Phi | H - E | \Phi \rangle = 0. \tag{8}$$

Variational principle (8) applied to the states from many-body Fock space

$$|\Phi\rangle = \sum_n \iiint dk_1 \dots dk_n C_{(i)}(k_1,\dots,k_n) a^\dagger_{k_1} \dots a^\dagger_{k_n} |0\rangle \tag{9}$$

typically leads to an infinite system of coupled equations for the amplitudes $C_{(i)}(k_1,\dots,k_n)$. This is usually simplified using Tamm-Dancoff truncation [5] or a variational ansatz [3]. Ansatzes involving a handful of few-body excitations, e.g.

$$|\Phi\rangle = (1 + \int dk f_k a^\dagger_k + \iint dk_1 dk_2 f_{k_1 k_2} a^\dagger_{k_1} a^\dagger_{k_2})|0\rangle,$$

are often used in addition to ansatzes defined by coherent states

$$|\Phi\rangle = \exp(\int dk f_k a^\dagger_k)|0\rangle \tag{10}$$

or

$$|\Phi\rangle = \exp(\iint dk_1 dk_2 f_{k_1 k_2} a^\dagger_{k_1} a^\dagger_{k_2})|0\rangle. \tag{11}$$

While variational approach in QFT retains such important features as simplicity in application and formulation as well as significant nonperturbative contents, it suffers from numerous drawbacks which hampered its applications in QFT. Among these is the lack of explicit covariance, the necessity of nonperturbative regularization/renormalization if the model is not a-priory finite and the growing complexity of trial quantum states. In this paper, we are going to consider a new variational approach that may be helpful in dealing with the latter problem.

We note that, while in Quantum Mechanics the quantum state could be described by a single wavefunction, in QFT one needs an infinite number of many-body amplitudes $C_{(i)}(k_1,\dots,k_n)$, as introduced in Eq.(9), to properly describe the quantum state. This makes general variational problem intractable and even simpler variational ansatzes, like in Eqs.(10) and (11), require significant algebraic work to obtain higher particle number contributions. In QFT, one has to deal with an infinite number of many-body amplitudes even though one may only need to compute a limited number of the relevant expectation values, e.g. $\langle\pi^2\rangle$, $\langle(\nabla\phi)^2\rangle$, $\langle\phi^2\rangle$, $\langle\phi^4\rangle$ in ϕ^4 scalar field theory. This overcomplicated nature of variational approach in QFT led us to the following idea. Instead of going through the complex Fock space representation of the trial quantum state in computing the expectation values of the relevant operators, one may parametrize the trial configuration in terms of the expectation values themselves, e.g. $\Delta_\pi = \langle\pi^2\rangle$, $\Delta_{\phi^2} = \langle\phi^2\rangle$ and $\Delta_{\phi^4} = \langle\phi^4\rangle$. Because of the quantum nature of operators, certain constraints would be imposed on the expectation values Δ's by quantum algebra. Then, the variational problem is cast into a constrained minimization problem in terms of only the relevant expectation values, e.g.

$$\begin{array}{l} \frac{1}{2}(\Delta_\pi + \Delta_{\nabla\phi} + m^2\Delta_{\phi^2}) + \frac{\lambda}{4!}\Delta_{\phi^4} \to \min \\ \text{constraints on } \Delta_\pi, \Delta_{\nabla\phi}, \Delta_{\phi^2}, \Delta_{\phi^4}. \end{array}$$

This idea is specifically motivated by the following theorem.

First Symmetric Decomposition Theorem: Symmetrized Fock space $\mathcal{F} = \{|\eta\rangle\}$ is isomorphic via

$$\langle\eta|a_k^\dagger a_{k'}|\eta\rangle = g(k,k')$$

to the space of linear integral operators with kernel $g(k,k')$ that are positive definite hermitian and have finite traces. By this we claim that, if $g(k,k')$ is known to define a hermitian positive definite linear integral operator with a finite trace, then there exists a normalized quantum state in symmetrized Fock space $\mathcal{F}$ which gives $g(k,k')$ as $\langle a_k^\dagger a_{k'}\rangle$ and vice versa.

To prove the First Symmetric Decomposition Theorem, we note that for hermitian operator introduced by kernel $g(k,k')$ there should exist a full orthonormal set of eigenfunctions and eigenvalues such that

$$g(k,k') = \sum_m \lambda_m g_m(k) g_m^*(k'), \tag{12}$$

where $g_m^*(k')$ is a complex conjugation of eigenfunction $g_m(k)$ and for positive definite operators the eigenvalues $\lambda_m \geq 0$. It is sufficient to consider a set of states

$$|n\rangle = \frac{1}{\sqrt{n!}} \iint dk_1 \ldots dk_n f_n^*(k_1,\ldots,k_n) a_{k_1}^\dagger \ldots a_{k_n}^\dagger |0\rangle, \tag{13}$$

where

$$f_n(k_1,\ldots,k_n) = \sum_m \sqrt{\lambda_m} g_m(k_1)\ldots g_m(k_n). \tag{14}$$

Given orthogonality and normalization of the eigenfunctions, it is easy to check that

$$\langle n|a_k^\dagger a_{k'}|n\rangle = \sum_m \lambda_m g_m(k) g_m^*(k') = g(k,k').$$

Then, it is always possible to choose a set of amplitudes β_n such that for $|\eta\rangle = \sum\limits_n \beta_n |n\rangle$

$$\langle\eta|a_k^\dagger a_{k'}|\eta\rangle = g(k,k') \text{ and } \langle\eta|\eta\rangle = 1.$$

Note that a finite trace is required provided that

$$\langle\eta|N|\eta\rangle = \mathrm{Tr}[g(k,k')] < \infty.$$

It is trivial to show that for any $|\eta\rangle$ from the Fock space the expectation value $\langle a_k^\dagger a_{k'}\rangle$ defines a positive definite hermitian linear integral operator with a finite trace. This completes the proof.

Furthermore, it is possible to extend this statement to **Second Symmetric Decomposition Theorem** stating that for expectation values on a normalized quantum state from symmetrized Fock space $|\eta\rangle$,

$$\begin{aligned} A_\eta(k,k') &= \langle\eta|a_k^\dagger a_{k'} + b_{-k'}^\dagger b_{-k}|\eta\rangle, \\ B_\eta(k,k') &= \langle\eta|a_k^\dagger b_{-k'}^\dagger + a_{k'} b_{-k}|\eta\rangle, \end{aligned} \tag{15}$$

treated as kernels of hermitian linear integral operators, precisely

$$1 + A_\eta \succeq \sqrt{1 + B_\eta^2}, \tag{16}$$

i.e. $1 + A_\eta - \sqrt{1 + B_\eta^2}$ is a positive definite operator[a].

The significance of these statements is in the claim that any expectation value of the form given above can be represented in terms of a state from the Fock space and vice versa. Thus, in dealing with these expectation values one need not an explicit complex structure from the Fock space but may work entirely in terms of the relevant expectation values constrained by a condition like in Eq.(16).

We will now illustrate application of this principle to the example of a study of ground state and critical phenomena in a variant of nonlinear sigma model. Advantage of this model for our application will be that it is completely formulated in terms of the expectation values of the quadratic operators in ϕ and, thus, our results about isomorphism between $\mathcal{F}$ and (A_η, B_η) can be straightforwardly applied. $O(N)$ nonlinear sigma model is introduced as a free field theory constrained to live on a sphere of radius R. It is defined by a free field Hamiltonian

$$H = \int dx \frac{1}{2}(\vec{\pi}^2 + (\nabla\vec{\phi})^2 + \mu^2\vec{\phi}^2) \tag{17}$$

and a constraint for N-component vector $\vec{\phi}(x)$

$$|\vec{\phi}(x)|^2 = R^2. \tag{18}$$

In our model we will enforce this constraint softly on average, so that in the canonical quantization Eqs.(17) and (18) will be given by

$$\begin{aligned} &\langle : H :\rangle \sim \int dk \epsilon_k \sum_i A_\eta^i(k,k) \\ &\langle : |\vec{\phi}^2(x)| :\rangle \sim \int dK dk \frac{e^{ixK}}{\sqrt{\epsilon_k \epsilon_{k+K}}} \sum_i [A_\eta^i(k, K+k) + B_\eta^i(k, K+k)] \end{aligned} \tag{19}$$

We define the physical subspace as the subset of the Fock space $\mathcal{F}$ satisfying condition $\langle\eta| : |\phi^2(x)| : |\eta\rangle = R^2$. Consequently, we define the ground state as the state from the physical subspace with the lowest energy.

We reformulate an original variational problem for the ground state in terms of the expectation values themselves, subject to the quantum algebra constraint (16). In these terms for the hermitian linear integral operators A_η and B_η, we have

$$\begin{cases} \mathrm{Tr}[\epsilon \cdot A_\eta^i] \to \min \\ \mathrm{Tr}[\epsilon^{-1} \cdot (A_\eta^i + B_\eta^i)] = R^2 \\ \text{off-diagonal} \int dk \frac{1}{\sqrt{\epsilon_k \epsilon_{K+k}}} \sum_i [A_\eta^i(k, K+k) + B_\eta^i(k, K+k)] = 0, \;\; K \neq 0. \end{cases} \tag{20}$$

Here ϵ is the diagonal matrix with $\epsilon_{kk'} = \sqrt{k^2 + \mu^2}\delta_{kk'}$, "$\cdot$" stands for matrix multiplication and Tr stands for integration over momenta and summation over i.

[a] note that $B_\eta^2 = \langle\eta|B|\eta\rangle\langle\eta|B|\eta\rangle \neq \langle\eta|B^2|\eta\rangle$ for $B = a^\dagger b^\dagger + ab$

From Eq.(16), we know that for given B_η^i linear operator A_η^i can be represented by $A_\eta^i = \mathcal{M}^i + \sqrt{1+(B_\eta^i)^2} - 1$, where $\mathcal{M}^i \succeq 0$. Then,

$$\begin{aligned} &\mathrm{Tr}[\epsilon \cdot A_\eta^i] \to \min \Leftrightarrow \\ &\mathrm{Tr}[\epsilon \cdot \mathcal{M}^i] + \mathrm{Tr}[\epsilon \cdot (\sqrt{1+(B_\eta^i)^2} - 1)] \to \min . \end{aligned} \tag{21}$$

Given $\mathcal{M} \succeq 0$, diagonal elements $\mathcal{M}_{k,k}^i \geq 0$ and $\mathrm{Tr}[\epsilon \cdot \mathcal{M}^i] \geq 0$ so that to minimize the expectation value of the Hamiltonian one needs obviously $\mathcal{M}^i \to 0$. Thus, the constraint Eq.(16) is resolved and we get

$$\begin{cases} \mathrm{Tr}[\epsilon \cdot (\sqrt{1+(B_\eta^i)^2} - 1)] \to \min \text{ (a)} \\ \mathrm{Tr}[\epsilon^{-1} \cdot (\sqrt{1+(B_\eta^i)^2} - 1 + B_\eta^i)] = R^2 \text{ (b)} \\ \int dk \frac{1}{\sqrt{\epsilon_k \epsilon_{K+k}}} \sum_i [\sqrt{1+(B_\eta^i)^2} - 1 + B_\eta^i](k, K+k) = 0, \; K \neq 0 \text{ (c)}. \end{cases} \tag{22}$$

One can observe that for the solution of Eqs.(22a) and (22b) B_η^i should be diagonal. For off-diagonal $k \neq k'$, one may consider variation $\delta B_{kk'}^i$ that preserves Eq.(22b) and show that

$$\delta \mathrm{Tr}[\epsilon \cdot (\sqrt{1+(B_\eta^i)^2} - 1)] = (1 - \frac{\epsilon_k^2}{\epsilon_{k'}^2}) \epsilon_{k'} \left(\frac{B_\eta^i}{\sqrt{1+(B_\eta^i)^2}} \right)_{k'k} \delta B_{kk'}^i , \tag{23}$$

which implies that B_η^i with off-diagonal nonzero elements cannot be the solution of the minimization problem (22). In that case Eq.(22c) is redundant as it is automatically satisfied by the solution of Eqs.(22a) and (22b).

Having said that, the problem defined by Eqs.(22a) and (22b) can be solved using the method of Lagrange multipliers. We introduce a new variable

$$Q_\eta^i(k) = \sqrt{1+(B_\eta^i(k,k))^2} - 1 + B_\eta^i(k,k), \tag{24}$$

and rewrite Eq.(22) in the form

$$\begin{aligned} &\sum_i \int dk \frac{[Q_\eta^i(k)]^2}{1+Q_\eta^i(k)} \epsilon_k \to \min \\ &\sum_i \int dk Q_\eta^i(k) \epsilon_k^{-1} = R^2, \end{aligned} \tag{25}$$

which is rewritten with Lagrange multiplier λ as

$$\begin{aligned} &\delta_{Q_\eta^i(k)} \sum_i \int dk \left(\frac{[Q_\eta^i(k)]^2}{1+Q_\eta^i(k)} \epsilon_k - \lambda Q_\eta^i(k) \epsilon_k^{-1} \right) = 0 \Rightarrow \\ &Q_\eta^i(k) = \frac{\epsilon_k}{\sqrt{\epsilon_k^2 - \lambda(R^2)}} - 1 \end{aligned} \tag{26}$$

and Eq.(25) is then given by

$$N \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{2\epsilon_k} \left[\frac{\epsilon_k}{\sqrt{\epsilon_k^2 - \lambda(R^2)}} - 1 \right] = R^2. \tag{27}$$

Eq.(27) is the gap-equation for $\lambda(R^2)$. In 2+1 dimensions, this integral can be computed exactly to yield

$$\frac{N\mu}{4\pi}\left(1-\sqrt{1-\frac{\lambda(R^2)}{\mu^2}}\right)=R^2. \tag{28}$$

Thus, we arrive at the following solution of our original problem. The ground state in our model, defined as the state from the Fock space $\mathcal{F}$ with lowest energy $\langle : H : \rangle$ and satisfying $\langle : |\phi^2(x)| : \rangle = R^2$, is described for $R^2 \leq R_c^2 = \frac{N\mu}{4\pi}$ by the expectation value $\langle : \phi_i(k)^* \phi_i(k) : \rangle = \frac{\epsilon_k}{\sqrt{\epsilon_k^2 - \lambda}} - 1$, where λ is the solution of Eq.(28). For $R^2 > R_c^2$ the solution of the form (26) can no longer be found because of the "finite capacity" of $k \neq 0$ modes in the distribution (26). Instead, the ground state is described as superposition of distribution (26) with $\lambda = \mu^2$ and a singular Bose condensation in $k = 0$ mode. Development of Bose condensation for $R^2 > R_c^2$ describes a phase transition of the second kind in this model.

This discussion is the exact variational solution of the original problem thanks to the exact constraints on the expectation values A_η and B_η that we were able to find. As one can see, we rendered the explicit Fock space structure completely unnecessary. The final answer was given in terms of the expectation values of a given operator on the ground state without explicit reference to the Fock space.

While the knowledge of an exact image of the Fock space $\mathcal{F}$ in terms of given expectation values, say A_η and B_η, is very interesting and, as we have shown, may be beneficial in certain problems, such detailed information for the expectation values of more complex operators, e.g. ϕ^4, may be difficult to obtain. In general, if approximate constraints on the expectation values of the operators can be established, the approach outlined above would provide a variational estimate for the ground state of the model. Among its advantages would be elimination of the necessity to include the consideration of complicated states from the Fock space explicitly as well as a possibility to incorporate renormalizations via the expectation values of the quantum operators themselves as they enter the final constrained optimization problem. In this sense further investigations of this approach present clear interest.

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