New Approach to the variational Method for the Quantum Field Theory: Example of Critical Phenomena in 2+1 Dimensional Nonlinear Sigma Model

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Introduction to Variational Method

Schrodinger Equation:

$$i\hbar \frac{\partial}{\partial t}\left|\Psi\right\rangle = H\left|\Psi\right\rangle$$

$$H = -\frac{\hbar^2}{2m^2}\nabla^2 + V(r)$$

Solutions of Schrodinger Equation

$$\left\{E_n, \left|\Psi_n\right\rangle\right\}$$

Introduction to Variational Method

- Solutions form full basis

$$|\Phi\rangle = \sum_n \varphi_n |\Psi_n\rangle$$

$$|\Phi, t\rangle = \sum_n \varphi_n e^{-i\frac{E_n t}{\hbar}} |\Psi_n\rangle$$

- Ritz Principle

$$\langle\Phi|H|\Phi\rangle = \sum_{n,n'} \varphi_n^* \varphi_{n'} \langle\Psi_n|H|\Psi_{n'}\rangle =$$

$$\sum_{n,n'} |\varphi_n|^2 E_n \langle\Psi_n|\Psi_n\rangle \geq E_0 \langle\Phi|\Phi\rangle$$

Introduction to Variational Method

Variational Principle

- if $\left\{ \left| \Phi_\alpha \right\rangle, \alpha \in A \right\}$ is a class of trial "*variational*" states
- if $E = \min\limits_{\alpha \in A} \frac{\left\langle \Phi_\alpha \middle| H \middle| \Phi_\alpha \right\rangle}{\left\langle \Phi_a \middle| \Phi_a \right\rangle}$
- then $E \geq E_0$

allows to estimate ground state energy in system

Introduction to Variational Method

- In Quantum Mechanics states $|\Psi\rangle$ are represented with wave-functions, e.g. in coordinate representation

$$|\Psi\rangle \propto \Psi(x)$$

- One considers a trial wave-function with few or many adjustable parameters

$$|\Phi_\alpha\rangle \propto \Phi(x;\alpha_1,\ldots,\alpha_m)$$

Introduction in Variational Method

Example: Hydrogen Atom

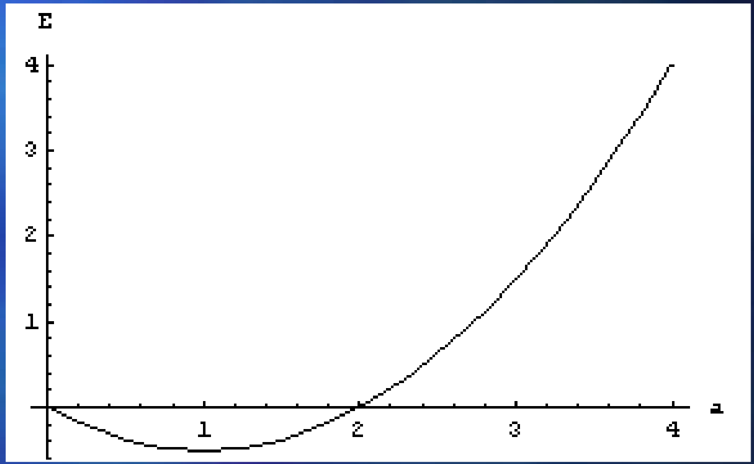
$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}$$

$$\Phi(r;\alpha) = e^{-\alpha r}$$

$$\frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \frac{a(a-2)}{2}$$

$$a = 1.0$$

$$E = -0.5$$

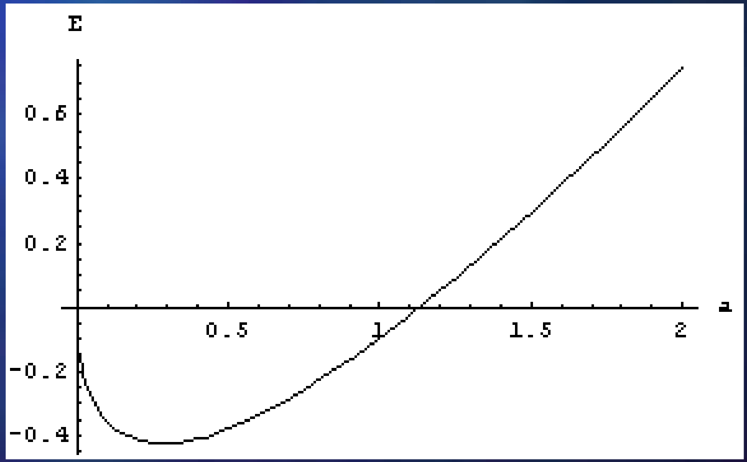


$$\Phi(r;\alpha) = e^{-\alpha r^2}$$

$$\frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \frac{3a}{2} - 2\sqrt{\frac{2a}{\pi}}$$

$$a = 0.2829...$$

$$E = -0.4244...$$



Introduction to Variational Method

PROS

- Nonperturbative analytical results
- Known upper energy estimate
- If trial states class is wide enough, may give exact answer

CANS

- Only as good as is the choice of trial states class
- Hard to control and estimate the error

Introduction to Variational Method

In Quantum Field Theory

$$P^{\mu} P_{\mu} \left| \Psi \right\rangle = M^{2} \left| \Psi \right\rangle$$

In Center of Mass Frame

$$P^{i} \left| \Psi \right\rangle = 0, i = 1,2,3$$

$$P^{0} P_{0} \left| \Psi \right\rangle = M^{2} \left| \Psi \right\rangle \Rightarrow$$

$$P^{0} \left| \Psi \right\rangle = \pm M \left| \Psi \right\rangle$$

normally choose positive energies (particles)

Introduction to Variational Method

In Schrodinger picture

$$\frac{\langle \Psi | P^0 | \Psi \rangle}{\langle \Psi | \Psi \rangle} = E(\Psi) \geq E_0$$

In QFT the Quantum State is much more complicated structure than in QM

$$|\Psi\rangle = \sum_{(i)} \iiint dx_1 ... dx_n C_{(i)}(x_1, ..., x_n) a^+_{i_1} ... a^+_{i_n} |0\rangle$$

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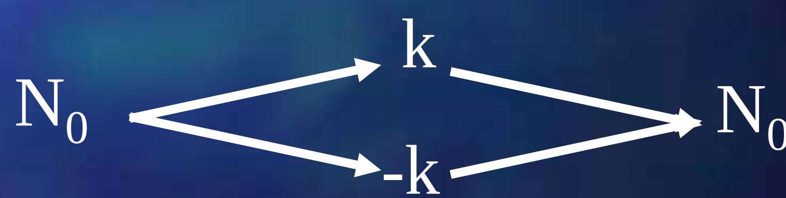
Example: superfluidity

$$H \approx \frac{1}{2}\sum_k \varepsilon_k^0 a_k^+ a_k + \frac{g}{2V}\left[N_0^2 + 2N_0 \sum_{k\neq 0}\left(a_k^+ a_{-k}^+ + 2a_k^+ a_k + a_k a_{-k}\right) + O(1)\right]$$

$$\Downarrow$$

$$H = \sum_k \varepsilon_k^0 a_k^+ a_k + \frac{1}{2V}\sum_{k_1\ldots k_4} V_{k_1-k_3}\, a_{k_1}^+ a_{k_2}^+ a_{k_3} a_{k_4}\, \delta_{k_1+k_2,k_3+k_4}$$

- *0-mode dominance* $\quad \left\langle a_0^+ a_0 \right\rangle = N_0 >> N - N_0 \qquad a_0 \approx \sqrt{N_0}$
- *short range* $\quad V(x) \approx g\delta(x)$
- *leading interaction in* $\frac{1}{N_0}$ *is 0-mode in/out scatterings*



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$$H \approx \frac{1}{2}\sum_k \varepsilon_k^0 a_k^+ a_k + \frac{g}{2V}\left[N_0^2 + 2N_0 \sum_{k\neq 0}\left(a_k^+ a_{-k}^+ + 2a_k^+ a_k + a_k a_{-k}\right)\right]$$

...diagonalizable with Bogoliubov transformation

$$\tilde{a}_k = u_k a_k - v_k a_{-k}^+$$

$$\tilde{a}_{-k}^+ = u_k a_{-k}^+ - v_k a_k$$

$$u_k^2 - v_k^2 = 1,\ k \neq 0$$

$$H \approx \frac{gn^2 V}{2} - \frac{1}{2}\sum_{k\neq 0}\left(\varepsilon_k^0 + ng - \sqrt{\left(\varepsilon_k^0\right)^2 + 2ng\varepsilon_k^0}\right) + \sum_{k\neq 0}\sqrt{\left(\varepsilon_k^0\right)^2 + 2ng\varepsilon_k^0}\,\tilde{a}_k^+ \tilde{a}_k$$

Introduction to Variational Method

Variational Approach in Field Theory

$$|\Omega\rangle = \exp\left(\int dk\ f(k) a_k^+ \right) |0\rangle$$

$$E = \min_{|\Omega\rangle} \frac{\langle \Omega | H | \Omega \rangle}{\langle \Omega | \Omega \rangle}$$

- *choose trial state in some form*
- *system of integral-differential equations*
- *(gap equation)*

Introduction to Variational Method

Variational Approach in QCD (BCS, TDA, RPA)

$$|\Omega\rangle = \exp\left(\int dk\ f(k) a_k^+ b_{-k}^+ - h.c.\right)|0\rangle$$

A form of Bogoliubov transformation

$$\varphi(\vec{x}) = \int \frac{d\vec{k}}{(2\pi)^3} \frac{1}{\sqrt{2\omega'_{\vec{k}}}} (A_{\vec{k}} + B_{-\vec{k}}^+) e^{i\vec{k}\cdot\vec{x}} = \int \frac{d\vec{k}}{(2\pi)^3} \frac{1}{\sqrt{2\omega_{\vec{k}}}} (a_{\vec{k}} + b_{-\vec{k}}^+) e^{i\vec{k}\cdot\vec{x}}$$

$$A_k = \cosh(\zeta_k) a_k - \sinh(\zeta_k) b_{-k}^+$$

$$B_k = \cosh(\zeta_k) b_k - \sinh(\zeta_k) a_{-k}^+$$

$\omega(k)$ [$\zeta(k)$] is subject to variation

Introduction to Variational Method

Advantages of Variational Method in QFT

- *possibility of nonperturbative results*
- *possibility of high numerical efficiency*

Difficulties of Variational Method in QFT

- *complicated general structure of Quantum States*
- *necessity of regularization/renormalization* *<u>nonperturbative</u> procedure if result is not finite*
- *only equal-time formulation*

Variational Method in QFT

Overcomplicated Quantum States structure

$$|\Psi\rangle = \sum_{(i)} \iiint dx_1 ... dx_n C_{(i)}(x_1, ..., x_n) a^+_{i_1} ... a^+_{i_n} |0\rangle$$

or even

$$|\Psi\rangle = \exp\left(\int dk \ f(k) a^+_k \right) |0\rangle$$

while, for example, in scalar ϕ^4 theory

$$P^0 = H = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{\lambda}{4}\phi^4$$

all we need is

$$\langle\Psi|\pi^2|\Psi\rangle, \langle\Psi|(\nabla\phi)^2|\Psi\rangle \ \ and \ \ \langle\Psi|\phi^4|\Psi\rangle$$

Variational Method in QFT

Guideline:

- *parameterize Quantum State in terms of expectation values themselves, e.g.*

  $\Delta_\pi \equiv \langle \Psi | \pi^2 | \Psi \rangle, \Delta_{\nabla\phi} \equiv \langle \Psi | (\nabla\phi)^2 | \Psi \rangle$ *and*

  $\Delta_{\phi^4} \equiv \langle \Psi | \phi^4 | \Psi \rangle$
- *derive constraints imposed on* Δ's *by quantum algebra*
- *obtain constrained minimization problem*

Variational Method in QFT

O(N) Nonlinear sigma model:

free field constrained to a sphere

$$H = \iint dx \frac{1}{2}\left(\vec{\pi}^2 + (\nabla\vec{\phi})^2 + \mu^2\vec{\phi}^2\right),$$

$$\left|\vec{\phi}(x)\right|^2 = R^2$$

can be rewritten in terms of ladder operators in Schrodinger picture

Variational Method in QFT

with

$$\phi(x) \propto \sum_i \iint dk \frac{1}{\sqrt{\varepsilon_k}} (\vec{\varepsilon}_i a_{ik} + \vec{\varepsilon}_i b^+_{-ik}) e^{ikx}$$

$$\pi(x) \propto \sum_i \iint dk\, i\sqrt{\varepsilon_k} (\vec{\varepsilon}_i b^+_{-ik} - \vec{\varepsilon}_i a_{ik}) e^{ikx}$$

one can get

$$: H :\propto \sum_i \iint dk \varepsilon_k (a^+_{ik} a_{ik} + b^+_{-ik} b_{-ik})$$

$$: \left|\vec{\phi}(x)\right|^2 :\propto$$

$$\sum_i \iint dk dk' \frac{e^{ix(k-k')}}{\sqrt{\varepsilon_k \varepsilon_{k'}}} (b^+_{-ik} a^+_{ik'} + a_{ik} b_{-ik'} + b^+_{-ik} b_{-ik'} + a^+_{ik'} a_{ik})$$

Variational Method in QFT

We intend to solve

$$\min\langle H\rangle \propto \min\sum_i \iint dk\varepsilon_k \langle a^+_{ik}a_{ik} + b^+_{-ik}b_{-ik}\rangle$$

subject

$$R^2 = \left\langle \left|\vec{\phi}(x)\right|^2 \right\rangle \propto$$

$$\sum_i \iint dk dk' \frac{e^{ix(k-k')}}{\sqrt{\varepsilon_k \varepsilon_{k'}}} \langle b^+_{-ik}a^+_{ik'} + a_{ik}b_{-ik'} + b^+_{-ik}b_{-ik'} + a^+_{ik'}a_{ik}\rangle$$

Variational Method in QFT

Theorem I:

for operator $a_k^+ a_{k'}$, Fock space $\mathcal{F} = \{|\eta\rangle\}$ and a kernel $g(k,k')$ of any *hermitian positive definite operator with finite trace,* in particular $g(k,k') = g^*(k',k)$, there exist $|\eta\rangle \in \mathcal{F}$ such that

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

Variational Method in QFT

If $g(k,k') = \sum_m \lambda_m g_m(k) g_m(k'),\ \lambda_m \geq 0$

sufficient to consider set of states

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

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

such that

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

Variational Method in QFT

$Tr[g(k,k')] < \infty$ is required for $\langle \eta | \mathbf{N} | \eta \rangle = Tr[g(k,k')] < \infty$

trivially for any $\eta \in \mathcal{F}$ $\langle \eta | a_k^+ a_{k'} | \eta \rangle$ is a hermitian, positive definite operator;

(!) Fock space is isomorphic to space of all hermitian, positive definite operators with finite trace

$$\mathcal{F} = \{ |\eta\rangle \} \propto$$

$$\mathcal{G} = \{ \text{hermitian, positive definite } g : C(\Re^n) \to C(\Re^n) \}$$

with finite trace

Variational Method in QFT

Similarly one can show that if

$$g(k,k') = \begin{pmatrix} g_{11}(k,k') & g_{12}(k,k') \\ g_{21}(k,k') & g_{22}(k,k') \end{pmatrix}$$

is kernel of hermitian, positive definite operator, then there exist $\eta \in \mathcal{F}$ such that

$$\langle \eta | A | \eta \rangle = \langle \eta \left| \begin{pmatrix} a_k^+ a_{k'} & a_k^+ b_{-k'}^+ \\ a_k b_{-k'} & b_{-k'}^+ b_{-k} \end{pmatrix} \right| \eta \rangle = \begin{pmatrix} g_{11}(k,k') & g_{12}(k,k') \\ g_{21}(k,k') & g_{22}(k,k') \end{pmatrix}$$

however, quantum states exist such that $\langle \eta | A | \eta \rangle$ *is not positive definite, thus not isomorphism*

Variational Method in QFT

In these terms our problem reads like

$$\min \sum_i \iint dk\varepsilon_k \left(g_{11}^{(i)}(k,k) + g_{22}^{(i)}(k,k)\right),$$

$$\sum_i \iint dkdk' \frac{e^{ix(k-k')}}{\sqrt{\varepsilon_k \varepsilon_{k'}}} \left(g_{11}^{(i)}(k,k') + g_{22}^{(i)}(k,k') + 2\,\mathrm{Re}\left[g_{12}^{(i)}(k,k')\right]\right) = R^2$$

to establish more precise constraints on $g_{lm}(k,k')$
consider Quantum Gaussian Packets

Variational Method in QFT

Quantum Gaussian Packet is a quantum state $|\alpha\rangle = U|0\rangle$ such that

$$U a_l U^+ = \sum_{l'} (\alpha_{ll'} a_{l'} + \beta_{ll'} a_{l'}^+)$$

Quantum Gaussian Packet can be built with

$$U^+ = V_\kappa^+ U_g^+ V_\kappa^+ \qquad U_g = \exp\left(-\frac{i}{2} \sum_{ll'} g_{ll'} \left[a_l^+ a_{l'}^+ + a_l a_{l'} \right] \right),$$

$$V_\kappa = \exp\left(-\frac{i}{2} \sum_{ll'} \kappa_{ll'} \left[a_l^+ a_{l'} + a_{l'} a_l^+ \right] \right)$$

Variational Method in QFT

using basic property of Quantum Gaussian Packets one can show that for averages

$$A_\eta = \langle \eta | a_k^+ a_{k'} + b_{-k'}^+ b_{-k} | \eta \rangle,$$

$$B_\eta = \langle \eta | a_k^+ b_{-k'}^+ + a_{k'} b_{-k} | \eta \rangle$$

and Quantum Gaussian Packet $|\alpha\rangle$

$$A_\alpha = \sqrt{1 + B_\alpha{}^2} - 1$$

Variational Method in QFT

furthermore, one can show that for any pare A and B such that

$$A = \mathcal{M} + \sqrt{1 + B^2} - 1,$$

$$\mathcal{M} \succ 0$$

there exist quantum state $\eta \in \mathcal{F}$ such that

$$A = A_\eta,$$

$$B = B_\eta$$

Variational Method in QFT

To know if

$$A_\eta \succ \sqrt{1+B_\eta{}^2} - 1$$

is an exact condition one need to show that Quantum Gaussian Packets provide absolute "minimum" for

$$1 + A_\eta - \sqrt{1+B_\eta{}^2}$$

Variational Method in QFT

We succeeded to show that

- QGP gives at least local extremum for this relation: $\delta_\eta\left(1+A_\eta-\sqrt{1+B_\eta^{\ 2}}\right)=0$
- QGP provide correct asymptotic form

$$A_\eta \succ \sqrt{1+B_\eta^{\ 2}}-1 \approx \left|B_\eta\right|-1,\ B_\eta - \text{large}$$

$$A_\eta \succ \sqrt{1+B_\eta^{\ 2}}-1 \approx \frac{B_\eta^{\ 2}}{2},\ B_\eta - \text{small}$$

Hypothesis: $A_\eta \succ \sqrt{1+B_\eta^{\ 2}}-1$ ***is exact constraint*** **(?)**

Variational Method in QFT

In these terms we translate for: $\begin{pmatrix} g_{11}(k,k') & g_{12}(k,k') \\ g_{21}(k,k') & g_{22}(k,k') \end{pmatrix}$

$$g_{12} = g_{21}^{+}, g_{11} \text{ and } g_{22} \text{ hermitian;}$$

$$g_{11}, g_{22} \succ \frac{1}{2}\left(\sqrt{1+\frac{(g_{12}+g_{21})^2}{4}}-1\right)$$

Variational Method in QFT

Example: O(N) nonlinear sigma model

$$E = \left\langle \iint dx \sum_i :\left(\pi_i^{\,2} + (\nabla\phi_i)^2\right): \right\rangle \to \min$$

$$\left\langle \sum_i :\phi_i^{\,2}: \right\rangle = \Delta$$

in terms of symmetric decomposition is

$$E = Tr[\sum_i \varepsilon \cdot A_{i,\eta}] \to \min$$

$$Tr[\sum_i \varepsilon^{-1} \cdot (A_{i,\eta} + B_{i,\eta})] = 2\Delta$$

Variational Method in QFT

To analyze this problem we introduce

$$Q_i = A_{i,\eta} + B_{i,\eta},$$

$$Q_i \succ \sqrt{1 + B_i^{\,2}} + B_i - 1$$

[diagonal part of] which leaves us with

$$E = Tr[\sum_i (\varepsilon \cdot Q_i - \varepsilon \cdot B_i)] \to \min,\ Tr[\sum_i \varepsilon^{-1} \cdot Q_i] = 2\Delta$$

$$Q_i \succ \sqrt{1 + B_i^{\,2}} + B_i - 1$$

Variational Method in QFT

Since Q and B enter independently, one shall clearly maximize B

$$E = \sum_i \iint dk \frac{Q_{i,k}^2}{1+Q_{i,k}} \varepsilon_k \to \min,$$

$$\sum_i \iint dk\, Q_{i,k} \varepsilon_k^{-1} = 2\Delta$$

Variational Method in QFT

solution: $Q_{i,k} = \frac{\varepsilon_k}{\sqrt{\varepsilon_k{}^2 - \lambda(\Delta)}} - 1,$

$$N \iint \frac{dk}{(2\pi)^{d-1}} \frac{1}{2\varepsilon_k} \left[\frac{\varepsilon_k}{\sqrt{\varepsilon_k{}^2 - \lambda(\Delta)}} - 1 \right] = \Delta$$

in 2+1 dimensions

$$N \iint \frac{dk}{(2\pi)^{d-1}} \frac{1}{2\varepsilon_k} \left[\frac{\varepsilon_k}{\sqrt{\varepsilon_k{}^2 - \lambda(\Delta)}} - 1 \right] = \frac{N\varepsilon_0}{4\pi} \left(1 - \sqrt{1 - \lambda(\Delta)} \right) = \Delta$$

$$\frac{N\mu}{4\pi} \geq \Delta$$

Variational Method in QFT

Existence of critical point can be well illustrated by separating explicitly 0-mode in Q

$$Q_0 = \varepsilon_0 (2\Delta - \iint_{k \neq 0} dk \frac{Q_k}{\varepsilon_k}),$$

$$E = \varepsilon_0 \frac{Q_0{}^2}{2 + 2Q_0} + \iint_{k \neq 0} dk \varepsilon_k \frac{Q_k}{2 + 2Q_k}$$

and is due to finite number of states $k \neq 0$ modes can support:

$$\iint_{k \neq 0} dk \frac{Q_k}{\varepsilon_k} < \infty$$

Variational Method in QFT

If Δ is too large, residual particles accumulate in 0-mode producing Bose-condensation

The order parameter, related to amount of condensation, develops continuously indicating 2nd order phase transition

Summary

- Presented novel approach to variational method in QFT*:*
  - *encode trial quantum state in terms of relevant expectation values*
  - *consider corresponding quantum-algebraic constraints*
  - *solve constrained optimization problem*
- Considered quantum operators relevant for O(N) nonlinear sigma model and constraints for their expectation values
- Presented complete solution for O(N) nonlinear model in 2+1 dimensions