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SCHRODINGER REPRESENTATION OF QUANTUM
FIELD THEORY

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**FUNCTIONALS HARTREE-FOCK
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Abstract

Following arguments used in quantum chemistry and many body theory, we derive the Hartree-Fock equations for a scalar field theory in the Schrodinger representation. We show that the renormalization of the total energy in the functional Schrodinger equation is entirely contained in the eigenvalues of the Hartree-Fock hamiltonian.

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Recently the Schrodinger representation of QFT has been discussed extensively in the literature [1].

The fundamental reason of this interest is the study of alternative points of view and to develop non-perturbative methods and new approximations schemes in QFT. The Schrodinger representation of QFT permits one to obtain more intuitive results following analogies with quantum mechanics and also to deduce straightforward aspects of topological interest in QFT [2].

In spite of the closed analogy between the Schrodinger representation of QFT and quantum mechanics, there exists various subtle points that have been noted in the literature [3]. These aspects make the Schrodinger representation of QFT fundamentally of quantum mechanics. The characteristic divergences in QFT appears in the Schrodinger representation approach in the zero point energy, in the presence of second functional derivatives evaluated in the same point and in the several non-equivalent Fock space that appears there.

These Fundamental problems have been treated partially in the literature and regularization and renormalization schemes [4-6] and prescriptions to choose the vacuum have been proposed [1].

The partial solution of these problems have permitted a coherent treatment of the Schrodinger representation of QFT at finite temperature [1], and by other hand, it opens the possibility of a systematic study of QFT.

Nevertheless in spite of this promisory results there are few approximations methods known to solve the functional Schrodinger equation and the proposit of this letter is to extend the well know Hartree-Fock formalism of quantum chemistry [7] and many body theory [8] to QFT. Our approach can be considered formal but we believe that our results can be of interest as a first step in systematic studies of the Hartree-Fock approximation in QFT.

The basic idea is to considerer a field theory with N scalar fields self-interacting coupled through a particular non-local interaction. We will show, using the variational method, that the minimal condition on the energy functional is that the Hartree-Fock equations are satisfied.

We consider the hamiltonian of the following scalar field theory:

$$H = \sum_{i=1}^N \int d^D x \left[-\frac{1}{2} \frac{\delta^2}{\delta \phi_i(x)^2} + \frac{1}{2} \nabla \phi_i \cdot \nabla \phi_i + V(\phi(x)) \right] +$$

$$+\frac{\mu_0}{2} \sum_{i=1}^N \sum_{j=1}^N \int d^D x d^D y \phi(x) G^{ij}(x, y) \phi_j(y) \quad (1)$$

where D is the spacetime dimension, μ_0 is a constant, $V(\phi_i(x))$ is an arbitrary polynomial in ϕ and $G^{ij}(x, y)$ is a non-local quantity that if we choose as $G^{ij}(x, y) = \delta^{ij} \delta(x, y)$, (1) will describe a local scalar field theory with $O(N)$ symmetry. Nevertheless, for generality, we suppose that $G^{ij}(x, y)$ is an arbitrary function symmetric in x and y .

The functional Schrodinger equation for this theory is :

$$H\Psi[\{\phi\}] = E\Psi[\{\phi\}] \quad (2)$$

where $\{\phi\} = \{\phi_1, \dots, \phi_N\}$.

The solutions of (2) give the complete quantum information about (1) and, of course, to obtain exact solutions of (2) is very difficult task.

Following the analogy with quantum mechanics, we consider approximate solutions of (2) by means of the variational method. The energy functional that we obtain from (2) is :

$$E[\{\phi\}] = \frac{\int D\phi_1 \dots D\phi_N \Psi[\{\phi\}]^* H\Psi[\{\phi\}]}{\int D\phi_1 \dots D\phi_N \Psi[\{\phi\}]^* \Psi[\{\phi\}]} \quad (3)$$

The next step is to choose an adequate trial wave functional and minimize (3). We will choose the following trial wave functional:

$$\Psi[\{\phi\}] = \Psi_1[\phi_1] \Psi_2[\phi_2] \dots \Psi_N[\phi_N] \quad (4)$$

which we suppose is normalized to one. i.e.,

$$\begin{aligned} \int D\phi_1 D\phi_2 \dots D\phi_N \Psi[\{\phi\}]^* \Psi[\{\phi\}] &= 1 = \\ &= \int D\phi_1 \Psi[\{\phi\}]_1^* \Psi[\{\phi\}]_1 \dots \int D\phi_N \Psi[\{\phi\}]_N^* \Psi[\{\phi\}]_N \end{aligned} \quad (5)$$

In practical calculations in quantum chemistry [7], it is necessary to give an ansatz for Ψ . In the same way, we will suppose that these functionals are gaussian ones [5,6].

Using (1), (5) and replacing (4) in (3), we obtain,

$$\begin{aligned} E[\{\phi\}] &= \sum_{i=1}^N \int D\phi_i \Psi[\phi_i] \int d^D x \left[-\frac{1}{2} \frac{\delta^2}{\delta\phi_i(x)^2} + \frac{1}{2} \nabla\phi_i \cdot \nabla\phi_i + V(\phi(x)) \right] \Psi[\phi_i] + \\ &+ \frac{\mu_0}{2} \sum_{i=1}^N \sum_{j=1}^N \int D\phi_i D\phi_j \Psi[\psi_i]^* \Psi[\psi_j]^* \int d^D x d^D y \phi_i(x) G^{ij}(x, y) \phi_j(y) \cdot \\ &\Psi[\phi_i] \Psi[\phi_j] \end{aligned} \quad (6)$$

The optimization condition of (6), is obtained by minimizing the functional (6) with the restriction (5), thus

$$\begin{aligned} \delta E + \epsilon_i \int D\phi_1 D\phi_2 \dots D\phi_i \dots D\phi_N \delta\Psi[\{\phi\}]^* \Psi[\{\phi\}] + \\ \epsilon_i \int D\phi_1 D\phi_2 \dots D\phi_i \dots D\phi_N \Psi[\{\phi\}]^* \delta\Psi[\{\phi\}] = 0 \end{aligned} \quad (7)$$

where the ϵ_i 's are Lagrange multipliers.

Calculating (7), we obtain the following result :

$$\begin{aligned} \sum_{i=1}^N \int D\phi_i \delta\Psi_i^*[\phi_i] \left(\int d^D x \left[-\frac{1}{2} \frac{\delta^2}{\delta\phi_i(x)^2} + \frac{1}{2} \nabla\phi_i \cdot \nabla\phi_i + V(\phi(x)) \right] \Psi_i[\phi_i] + \right. \\ \left. + \mu_0 \sum_{j=1}^N \int D\phi_j \Psi_j^*[\phi_j] \int d^D x d^D y \phi_j(x) G^{ij}(x, y) \phi_j(y) \Psi_j[\phi_j] \Psi_i[\phi_i] - \right. \\ \left. - \epsilon_i \Psi_i[\phi_i] \right) + \\ + \sum_{i=1}^N \int D\phi_i \delta\Psi_i[\phi_i] \left(\int d^D x \left[-\frac{1}{2} \frac{\delta^2}{\delta\phi_i(x)^2} + \frac{1}{2} \nabla\phi_i \cdot \nabla\phi_i + V(\phi(x)) \right] \Psi_i^*[\phi_i] + \right. \\ \left. + \mu_0 \sum_{j=1}^N \int D\phi_j \Psi^*[\phi_j] \int d^D x d^D y \phi_j(x) G^{ij}(x, y) \phi_i(y) \Psi_j[\phi_j] \Psi_i^*[\phi_i] - \right. \\ \left. - \epsilon_i^* \Psi_i^*[\phi_i] \right) = 0 \end{aligned} \quad (8)$$

The vanishing of (8), imply that:

$$\int d^D x \left[-\frac{1}{2} \frac{\delta^2}{\delta \phi_i(x)^2} + \frac{1}{2} \nabla \phi_i \cdot \nabla \phi_i + V(\phi(x)) \Psi_i[\phi_i] + \right. \\ \left. + \mu_0 \sum_{j=1}^N \int D\phi_j \Psi_j^*[\phi_j] \int d^D x d^D y \phi_j(x) G^{ij}(x, y) \phi_j(y) \Psi_j[\phi_j] \Psi_i[\phi_i] = \right. \\ \left. = \epsilon_i \Psi_i[\phi_i] \right] \quad (9)$$

$$\int d^D x \left[-\frac{1}{2} \frac{\delta^2}{\delta \phi_i(x)^2} + \frac{1}{2} \nabla \phi_i \cdot \nabla \phi_i + V(\phi(x)) \Psi_i^*[\phi_i] + \right. \\ \left. + \mu_0 \sum_{j=1}^N \int D\phi_j \Psi^*[\phi_j] \int d^D x d^D y \phi_j(x) G^{ij}(x, y) \phi_i(y) \Psi_j[\phi_j] \Psi_i^*[\phi_i] = \right. \\ \left. = \epsilon_i^* \Psi_i^*[\phi_i] \right] \quad (10)$$

The equations (9) and (10) are the minimization condition for the energy functional (6). This equations are the field theory extension of Hartree-Fock equations of quantum chemistry and many body theory. It is easy to show that the Hartree-Fock hamiltonian is hermitian and ,as consequence $\epsilon_i^* = \epsilon_i$.

The analogous of Koopman theorem [9] for QFT is obtained multiplying (9) by $\Psi[\phi_i]^*$, integrating in ϕ_i , and suming in i . The result is :

$$E[\{\phi\}] + \frac{\mu_0}{2} \sum_{i=1}^N \sum_{j=1}^N \int D\phi_i D\phi_j \Psi_i^*[\phi_i] \Psi_j^*[\phi_j].$$

$$\int d^D x d^D y \phi_i(x) G^{ij}(x, y) \phi_j(y) \Psi_i[\phi_i] \Psi_j[\phi_j] = \sum_{i=1}^N \epsilon_i \quad (11)$$

Note that when the non-local interaction is switched off ($\mu_0 \rightarrow 0$), the "energies" of the fields ϕ_i can be expressed completely in terms of the total energy E, thus the renormalization of ϵ_i in a local QFT is equivalent to the renormalization of E.

Of course, the problem of how to renormalize this theory is an open problem, perhaps using the methods proposed in the references [4-6], this can be solved.

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