Variational Approaches to the Dynamics of Mixed Quantum States

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Abstract. The time-dependent Schrödinger equation could be derived starting from the Dirac–Frenkel variational principle for the Dirac action $\int dt \langle \Psi(t)|i\hbar\frac{\partial}{\partial t} - H|\Psi(t)\rangle$. Restricting the variational space one can obtain different approximations. For instance one can obtain the time-dependent-Hartree–Fock approximation (TDHF) if the variational space is restricted to states which can be written as single Slater determinants. We discuss an approach based on the quantum variational principle which works also for mixed quantum states, states which are described by a density operator. We use the formalism of thermo field dynamics proposed by Umezawa to describe the mixed quantum states as pure states in a larger Hilbert space and we apply the Dirac–Frenkel variational principle in this space. In this way, using restricted variational states which have the form of vacuum states for Bogoliubov quasiparticles in the full Hilbert space (which mix not only creation and annihilation operators for physical degrees of freedom, but also creation and annihilation operators for unphysical degrees of freedom introduced in the formalism of thermo field dynamics) one can derive time-dependent-Hartree–Fock–Bogoliubov type of equation for mixed states. We illustrate this approach in detail for a single bosonic degree of freedom and we comment on the possibilities to use it for description of systems with an infinite number of degrees of freedom.

1 Introduction

A transport description of many-body non-equilibrium systems is a very convenient approximation used with success in the study of heavy ion collisions in the last two decades [1,2]. It is also used in the solid state physics to describe the transport properties like electric conductivity, thermal conductivity, etc, for more than 40 years. In this approach the one-body phase-space distribution function satisfies a semi-classical transport equation of Boltzmann type. The validity of the transport description can be established by a rigorous derivation from quantum field theory [3].

The dynamical evolution of a many-body system can be described, depending on the problem, either by classical mechanics or by quantum mechanics (quantum field theory being the quantum mechanics of classical fields). The classical mechanics for mixed states, neglecting the two-particle correlations, results in the celebrated Boltzmann equation for the phase-space one-particle distribution function. The conditions to use classical mechanics are not fulfilled for nucleons in a nucleus. Nevertheless, the Boltzmann-like equation was proven to be useful in the description of heavy ion collisions.

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There are two different ways to derive useful approximations for quantum systems. One way is to work in the Heisenberg picture (all the time dependence is included in time-dependent operators). Then, the standard perturbation expansion results into the Dyson equation for the one-particle Green functions. Further approximations result into a transport equation of Boltzmann type [3] (Boltzmann–Uehling–Uhlenbeck equation with collision term which takes into account the Pauli exclusion principle for fermions).

The other way is to work in the Schrödinger picture of quantum mechanics and to use judiciously chosen restricted trial states in the Dirac–Frenkel variational principle equivalent to the time-dependent Schrödinger equation. The problem is that this variational principle works only for pure states and we expect that in practice the state of the system would be more correctly approximated by a mixed state. Let us mention that there is a variational principle for the time evolution of a quantum density matrix in the literature [4], but the resulting equations for the approximate dynamical evolution of the system between time t_1 and time t_2 depend on the observable we want to calculate and they should be solved in general with both initial (at t_1) and final (at t_2) conditions and not as simple evolution equations with initial conditions.

In what follows we use the thermo field dynamics [5] to describe the mixed states as pure states in an enlarged Hilbert space. In this way the machinery of the Dirac–Frenkel variational principle could be used to derive approximations also for the time-evolution of mixed states, which are important for all the physical systems far from equilibrium.

The paper is organized as follows. First we will present the basic results of the time-dependent variational principle. Then we will discuss the description of mixed states as pure ones as it is realized in the formalism of thermo field dynamics. These results are used to construct a Lagrangian description for the parameters of some trial states; the trial states are chosen as vacuum states for Bogoliubov quasiparticles in the full Hilbert space of thermo field dynamics. Then we will discuss how the Lagrangian dynamics can be reformulated in the Hamiltonian form with a noncanonical Poisson bracket. In the next section we particularize the results to a simple example and we end with a discussion about the application of this treatment to problems in field theory.

2 Time-Dependent Variational Principle for Pure Quantum States

In the Schrödinger picture of quantum mechanics, in which the state (a vector in the Hilbert space of the system) depends on time and the observables (linear operators on the Hilbert space) are time independent, the time evolution of a pure state is given by the time-dependent Schrödinger equation

$$i\frac{d}{dt}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle \ , \tag{1}$$

where H is the Hamiltonian and $|\Psi(t)\rangle$ is the normalized many-body state which describes the physical system. This equation of motion can be obtained from the variation of the action [6–9]

$$A = \int_{t1}^{t2} dt \, \langle \Psi(t)| \, i\frac{d}{dt} - H \, |\Psi(t)\rangle \ . \tag{2}$$

This is the Dirac–Frenkel variational principle. In general, the set $|\Psi(t)\rangle$ contains infinitely many dynamical degrees of freedom, for example the complex coefficients of an orthonormal basis in the Hilbert space.

The advantage of the reformulation of the Schrödinger equation as a variational principle is the possibility that a suitably chosen restriction in the dynamical variables will lead to an useful approximation of the full problem. For instance, in the case of n fermions, one can obtain the time-dependent-Hartree–Fock approximation (TDHF) if the variational n-body space is restricted to states which can be written as single Slater determinants formed with n orthonormal one-body states [10], or one can obtain the Fermionic Molecular Dynamics (FMD) if the many-body trial state is a Slater determinant formed from n (nonorthogonal) one-body Gaussian wave packets [11]. In TDHF the dynamical variables are the n one-body states and in FMD the dynamical variables are the mean positions, mean momentums and complex widths of the n Gaussian wave packets.

From the action given by Eq. (2), and some restriction of the dynamical variables one can see that the time evolution of the system is a classical one for a system with the Lagrangian

$$\mathcal{L} = \langle \Psi(t)| \, i\frac{d}{dt} \, |\Psi(t)\rangle - \mathcal{H} \ , \tag{3}$$

where $\mathcal{H}$ is the expectation value of the quantum Hamiltonian

$$\mathcal{H} = \langle \Psi(t)| \, H \, |\Psi(t)\rangle \ . \tag{4}$$

The Lagrangian is a function of the usually complex dynamical variables $\Psi(t)$, so that $\Psi(t)$ and $\Psi^*(t)$ may be regarded as independent variables.

Before to discuss how the variational principle works with some particular trial states, we want to present a way to describe the mixed quantum states (states given by a density operator) as pure states. In this way we can use the Dirac–Frenkel variational principle to obtain variational approximations for systems in mixed states, too.

3 Mixed Quantum States and Thermofield Dynamics

In the formalism of thermo field dynamics [5,2] a mixed state is described as a pure state, the price to be paid for that being a doubling of the number of degrees of freedom. The idea is to consider the density operator, ρ, as

a vector in the Liouville space (the Liouville space is the vector space of linear operators acting on the Hilbert space of quantum system). Therefore, the Liouville space is the direct product of two copies of the Hilbert space of the system. We consider that the algebra of operators acting on the Hilbert space is generated by the creation and annihilation operators $a^\dagger$, a satisfying the commutation or anticommutation relations

$$\begin{aligned} a\, a^\dagger \mp a^\dagger a &= 1\,, \\ a\, a \mp a\, a &= 0\,, \\ a^\dagger a^\dagger \mp a^\dagger a^\dagger &= 0\,, \end{aligned} \tag{5}$$

depending on the bosonic or fermionic character of the considered system. In this case the algebra of operators acting on the Liouville space is generated by two commuting (for bosons) or anticommuting (for fermions) copies of the physical creation and annihilation operators, $a^\dagger$, a, denoted $a^\dagger$, a and $\tilde{a}^\dagger$, $\tilde{a}$. The vector in the Liuoville space is denoted $||\Psi\rangle\rangle$ and one of the main results of thermo field dynamics is that the time evolution of the state $||\Psi\rangle\rangle$ is given by a Schrödinger equation

$$i\frac{d}{dt}\,||\Psi(t)\rangle\rangle = \underline{H}\,||\Psi(t)\rangle\rangle\ , \tag{6}$$

with

$$\underline{H} = H(a^\dagger, a) - H(\tilde{a}^\dagger, \tilde{a})\ , \tag{7}$$

$H(a^\dagger, a)$ being the Hamiltonian of the system expressed in terms of the creation and annihilation operators. Therefore, instead to work with the density operator, $\rho(t)$, we can work equivalently with the pure state $||\Psi(t)\rangle\rangle$. The above evolution equation is equivalent to the quantum Liouville equation for the density matrix, ρ, and the expectation value of an operator O is given by its matrix element

$$\langle O\rangle = \langle\langle\Psi||\, O\,||\Psi\rangle\rangle \tag{8}$$

instead of $\mathrm{Tr}(\rho O)$. To illustrate the correspondence between the description by density matrix and the pure state description in Liouville space we give the correspondence between the density matrix for thermally equilibrated systems with one degree of freedom and the pure state in thermo field dynamics. For a non-interacting bosonic system the density matrix (not normalized) is

$$\rho \sim \mathrm{e}^{\frac{1}{k_B T}\, a^\dagger a}\ , \tag{9}$$

where k_B is the Boltzmann constant and T is the temperature of the system and the corresponding pure state in the thermo field dynamics is [5]

$$||\Psi\rangle\rangle \sim \mathrm{e}^{\mathrm{arcsinh}\left(\mathrm{e}^{\frac{1}{k_B T}}-1\right)^{-\frac{1}{2}}\, a^\dagger \tilde{a}^\dagger}\, ||0\rangle\rangle\ , \tag{10}$$

where $||0\rangle\rangle$ is the vacuum state in the Liouville space annihilated by the operators a and $\tilde{a}$. In the case of a non-interacting fermionic system with one degree of freedom we have the same density matrix, Eq. (9), (now the creation and annihilation operators will satisfy anticommutation relations) and the corresponding pure state is [5]

$$||\Psi\rangle\rangle \sim \mathrm{e}^{\arcsin\left(\mathrm{e}^{\frac{1}{k_B T}}+1\right)^{-\frac{1}{2}} a^\dagger \tilde{a}^\dagger} ||0\rangle\rangle \ . \tag{11}$$

We remark that the above states are annihilated by certain linear combinations of a and $\tilde{a}^\dagger$ and respectively $\tilde{a}$ and $a^\dagger$. In this sense the thermal equilibrated states are vacuum states for some special Bogoliubov quasiparticles named "thermal quasiparticles". The Bogoliubov transformation depend on temperature and does not mix only the creation and annihilation operators for physical particles, $a^\dagger$ and a, but also the creation and annihilation operators for unphysical particles, $\tilde{a}^\dagger$ and $\tilde{a}$, introduced in thermo field dynamics.

The above picture can be extended to a finite number, M, of fermionic or bosonic operators $a_\alpha^\dagger$ and a_α, $\alpha = 1, \ldots, M$ by introducing the operators $\tilde{a}_\alpha^\dagger$ and $\tilde{a}_\alpha$, $\alpha = 1, \ldots, M$.

To summarize this section, the description of a mixed state can be realized in the same way as for a pure state if we use $N = 2M$ creation and annihilation operators denoted by $A_i^\dagger$, A_i, $i = 1, \ldots, N$, where the set of operators A_i include a_α and $\tilde{a}_\alpha$.

Inspired by the form of thermal states, Eqs. (10, 11), we will use trial states which are annihilated by arbitrary linear combinations of the operators A_i and $A_i^\dagger$ (see Eq. (13) below).

4 Trial States and Classical Lagrange Dynamics

Let us consider a system described in terms of an arbitrary finite number, N, of creation and annihilation operators $A_i^\dagger$, A_i satisfying the commutation or anticommutation relations

$$\begin{aligned} A_i A_j^\dagger \mp A_j^\dagger A_i &= \delta_{ij} \ , \\ A_i A_j \mp A_j A_i &= 0 \ , \\ A_i^\dagger A_j^\dagger \mp A_j^\dagger A_i^\dagger &= 0 \ , \end{aligned} \tag{12}$$

where the upper sign refers to bosons and the lower one to fermions.

We choose a restricted class of variational states which have the form of a coherent superposition of $0, 2, 4, \cdots$ particle number components

$$|Z\rangle = \mathrm{e}^{\frac{1}{2} Z_{ij} A_i^\dagger A_j^\dagger} |0\rangle \ , \tag{13}$$

where $|0\rangle$ is the normalized vacuum state for fermionic or bosonic operators satisfying

$$A_i |0\rangle = 0 \ , \tag{14}$$

and Z is a skew symmetric complex matrix for fermions and a symmetric complex one for bosons and it parameterizes the trial state. The Einstein convention of summation over repeated indices is used. Our goal is to obtain equations for the time evolution of this variable. As the system was assumed to have an arbitrary finite number of degrees of freedom, N, Z is a $N \times N$ matrix and only at the end we allow N to become infinity.

When we want to describe pure states only, the operators $A_i^\dagger$ and A_i are the physical creation and annihilation operators of the system. The generalization to mixed states is simply done by doubling the dimension of the matrix Z which parameterizes the trial state.

The trial state given by Eq. (13) is the most general state which is not orthogonal to the vacuum in the fermionic case [10] (Thouless theorem). It is annihilated by certain linear combination of creation and annihilation operators and in this sense it can be considered as a vacuum for Bogoliubov quasiparticles. It is extensively used in time-independent problems in solid state and nuclear physics, mainly in the pure state (zero temperature) approximation, but it was not used in the time-dependent case.

Although it is not an eigenstate of the particle number operator and the Hamiltonian in the fermionic case conserves the number of particles, this is not a problem in practice for time-independent problems (e.g. BCS or Hartree–Fock–Bogoliubov calculations for nuclear structure) because, imposing a mean particle number, the particle number fluctuations are proven to be small; they are completely negligible in condensed matter physics. Moreover, when the particle number is small and one cannot neglect the unphysical particle number fluctuations introduced by such a trial state there are methods to retain only the component with the correct particle number by projecting the above trial state on a subspace of the Hilbert space [10,12–14]. We will not discuss such projection techniques in what follows. We want to stress that, as the above trial state is a superposition of components with $0, 2, 4, \cdots$ particles, it is useful for the description of systems with an even number of particles; the systems with an odd number of particles could be described using 1-particle excitations of the considered quasiparticle vacuum [10,15].

In the bosonic case there is a possibility to use a coherent state as trial state, too; it will be also a vacuum for some quasiparticles [10], but we restrict ourselves in the following to the above form.

The quantum state given by Eq. (13) is not normalized to unity and, before we can proceed further, we need to calculate its norm. Let us consider the complex valued function $\mathcal{F}(\xi)$ of a real variable ξ given by

$$\mathcal{F}(\xi) = \langle \xi \cdot Z_1 | Z_2 \rangle \ , \tag{15}$$

which reduces to $\langle Z_1 | Z_2 \rangle$ for $\xi = 1$ and when $Z_1 = Z_2 = Z$ it gives the norm of the state $|Z\rangle$. Taking into account the form of the trial state given by Eq. (13) one can see that $\mathcal{F}(0) = 1$ due to the normalization of the vacuum to unity. To calculate $\mathcal{F}(1)$ we use a trick to obtain a first order differential equation

for the function $\mathcal{F}(\xi)$. The solution of this differential equation which satisfies $\mathcal{F}(0) = 1$ will results into the overlap between two considered trial states, in particular into the norm of the state. Using the form of the hermitian adjoint of the state $|Z\rangle$

$$\langle Z| = \langle 0| \, \mathrm{e}^{\frac{1}{2} Z^*_{ij} A_j A_i} = \langle 0| \, \mathrm{e}^{\frac{1}{2} (Z^\dagger)_{ij} A_i A_j} \, , \tag{16}$$

where $*$ denotes complex conjugation and $\dagger$ denotes the adjoint of a matrix (transpose plus complex conjugation), one can write

$$\frac{d\mathcal{F}(\xi)}{d\xi} = \frac{1}{2} (Z_1^\dagger)_{ij} \, \langle \xi \cdot Z_1| \, A_i A_j \, |Z_2\rangle \, . \tag{17}$$

Using the commutation or anticommutation relations for creation and annihilation operators, Eq. (12), and the properties of the vacuum, Eq. (14), one obtains

$$A_j \, |Z\rangle = Z_{jk} A_k^\dagger \, |Z\rangle \, , \tag{18}$$

$$\langle Z| \, A_k^\dagger = \langle Z| \, A_l (Z^\dagger)_{lk} \, . \tag{19}$$

From the above two relations and the commutation relations for creation and annihilation operators, Eq. (12), we get

$$\begin{aligned} \pm \langle Z_1| \, A_j A_i \, |Z_2\rangle &= \langle Z_1| \, A_i A_j \, |Z_2\rangle \\ &= (Z_2)_{jk} \, \langle Z_1| \, A_i A_k^\dagger \, |Z_2\rangle \\ &= (Z_2)_{ji} \, \langle Z_1 | Z_2\rangle \pm (Z_2)_{jk} \, \langle Z_1| \, A_k^\dagger A_i \, |Z_2\rangle \\ &= (Z_2)_{ji} \, \langle Z_1 | Z_2\rangle \pm (Z_2)_{jk} (Z_1^\dagger)_{lk} \, \langle Z_1| \, A_l A_i \, |Z_2\rangle \\ &= (Z_2)_{ji} \, \langle Z_1 | Z_2\rangle + (Z_2 Z_1^\dagger)_{jl} \, \langle Z_1| \, A_l A_i \, |Z_2\rangle \, , \end{aligned}$$

where the upper sign refers to bosons and the lower one to fermions and in the last line the symmetry or skew symmetry of the Z matrix was used. Therefore, we have

$$(\mathbf{1} \mp Z_2 Z_1^\dagger)_{jl} \, \langle Z_1| \, A_l A_i \, |Z_2\rangle = \pm (Z_2)_{ji} \, \langle Z_1 | Z_2\rangle \, ,$$

from which, multiplying by $(\mathbf{1} \mp Z_2 Z_1^\dagger)_{kj}$ and replacing the indices k, i by i, j, we obtain

$$\langle Z_1| \, A_i A_j \, |Z_2\rangle = \pm \left((\mathbf{1} \mp Z_2 Z_1^\dagger)^{-1} Z_2 \right)_{ij} \, \langle Z_1 | Z_2\rangle \, . \tag{20}$$

The above relation for Z_1 replaced by $\xi \cdot Z_1$ is now used in Eq. (17) and with the appropriate symmetry of the matrix Z we obtains the following first order differential equation

$$\frac{d\mathcal{F}(\xi)}{d\xi} = \frac{1}{2} \mathrm{Tr} \left[Z_2 Z_1^\dagger \left(\mathbf{1} \mp \xi Z_2 Z_1^\dagger \right)^{-1} \right] \mathcal{F}(\xi) \, , \tag{21}$$

where Tr denotes the trace of a matrix and the cyclic permutation invariance of the trace was used.

The solution of this differential equation satisfying $\mathcal{F}(0) = 1$ is given by a simple integration

$$\begin{aligned}\mathcal{F}(\xi) &= \mathrm{e}^{\mp\frac{1}{2}\mathrm{Tr}\left[\ln\left(\mathbf{1}\mp\xi Z_2 Z_1^\dagger\right)\right]} \\ &= \mathrm{e}^{\mp\frac{1}{2}\mathrm{Tr}\left[\ln\left(\mathbf{1}\mp\xi Z_1^\dagger Z_2\right)\right]} \,. \end{aligned} \tag{22}$$

The equivalence of the above two forms can be established by using the power expansion of the logarithmic function and the invariance of the trace of a product with respect to a cyclic permutation of the factors. Therefore, the overlap of two trial states is

$$\langle Z_1 | Z_2 \rangle = \mathrm{e}^{\mp\frac{1}{2}\mathrm{Tr}\left[\ln\left(\mathbf{1}\mp Z_1^\dagger Z_2\right)\right]} \,, \tag{23}$$

which in the fermionic case is known as Onishi formula [10,16]. The norm of the state given by Eq. (13) is therefore

$$\langle Z | Z \rangle = e^{\mp\frac{1}{2}\mathrm{Tr}\left[\ln\left(\mathbf{1}\mp Z^\dagger Z\right)\right]} \,. \tag{24}$$

Using Eq. (20) we have the following expectation values

$$\frac{\langle Z | \, A_i A_j \, | Z \rangle}{\langle Z | Z \rangle} = \pm \left(Z(\mathbf{1} \mp Z^\dagger Z)^{-1} \right)_{ij} \,, \tag{25}$$

Taking the hermitian conjugate of the above relation we get

$$\frac{\langle Z | \, A_i^\dagger A_j^\dagger \, | Z \rangle}{\langle Z | Z \rangle} = \pm \left((\mathbf{1} \mp Z^\dagger Z)^{-1} Z^\dagger \right)_{ij} \,, \tag{26}$$

and using Eq. (18) it is a simple exercise to obtain

$$\frac{\langle Z | \, A_i^\dagger A_j \, | Z \rangle}{\langle Z | Z \rangle} = \pm \left[(\mathbf{1} \mp Z^\dagger Z)^{-1} - \mathbf{1} \right]_{ij} \,. \tag{27}$$

The expectation values of products of an even number, larger than two, of creation and annihilation operators can be obtained by taking the partial derivatives of the Eq. (23) with respect to the elements of matrix Z_1 or/and Z_2, using the commutation relations, Eq. (12), and properties of the trial state, Eq. (18), and at the end the result is written for $Z_1 = Z_2 = Z$. The expectation value of products of an odd number of creation and annihilation operators vanishes for trial state (13). In this way we can calculate $\mathcal{H}(Z, Z^\dagger)$ as the Hamiltonian of the system is given in terms of products of creation and annihilation operators.

To calculate the Lagrangian given by Eq. (3) with the trial states of the form written in Eq. (13) we need to use normalized states and the first term in Eq. (3) will be

$$\langle Z | \, \frac{1}{\langle Z | Z \rangle^{1/2}} i \frac{d}{dt} \frac{1}{\langle Z | Z \rangle^{1/2}} \, | Z \rangle \,,$$

with $\langle Z|Z\rangle$ given by Eq. (24). The time derivative of the norm will result in a term which is a total time derivative and is irrelevant in the Lagrangian, so the contribution of the above term to the Lagrangian can be written as

$$\frac{1}{\langle Z|Z\rangle}\langle Z|\, i\frac{d}{dt}\,|Z\rangle \ .$$

Now we can use the form of the trial state, Eq. (13), and the above contribution can be expressed as

$$\frac{1}{2}\frac{dZ_{ij}}{dt}\frac{\langle Z|\, A_i^\dagger A_j^\dagger\,|Z\rangle}{\langle Z|Z\rangle} \ .$$

With the expectation value given in Eq. (26) we can write the Lagrangian in the form

$$\begin{aligned}\mathcal{L} &= \pm i\frac{1}{2}\left((\mathbf{1}\mp Z^\dagger Z)^{-1}\right)_{ik} Z_{kj}^\dagger \frac{dZ_{ij}}{dt} - \mathcal{H}(Z,Z^\dagger) \\ &= i\frac{1}{2}\mathrm{Tr}\left[(\mathbf{1}\mp Z^\dagger Z)^{-1}Z^\dagger\frac{dZ}{dt}\right] - \mathcal{H}(Z,Z^\dagger)\ . \end{aligned} \tag{28}$$

Therefore, the quantum dynamical problem was reformulated as classical Lagrange dynamics for the parameters of the trial state. We want to stress that this approach works for pure states as well as for mixed states, but the dimension of the configuration space is larger in the second case.

5 Phase Space, Poisson Bracket and Hamilton Dynamics

We restrict in this section to the fermionic case, as the bosonic case can be studied along the same lines. First we remark that the Lagrangian (28) is first order in the time derivatives and the standard definitions of the conjugate momenta $P_{ij} = \frac{\partial\mathcal{L}}{\partial\frac{dZ_{ij}}{dt}}$ result into constraint equations in the associated phase space. This means that the phase space can be identified with the configuration space, but the Poisson brackets will be not in the canonical form. To approach this problem we can use the general method of Dirac to take into account the constraints by using them to replace the canonical Poisson bracket by a noncanonical one. In our particular case we can obtain directly the Poisson bracket as follows: the independent coordinates in the configuration space are Z_{ij}, for $j > i$ and their conjugate momenta are

$$P_{ij} = i\left[(\mathbf{1}+Z^\dagger Z)^{-1}Z^\dagger\right]_{ij}\ . \tag{29}$$

We mention that the other matrix elements of Z are not independent since $Z_{ij} = -Z_{ji}$. Therefore, we have the following Poisson bracket between coordinates and associated momenta

$$\{Z_{mn}, P_{ij}\} = \{Z_{mn}, i(\mathbf{1}+Z^\dagger Z)^{-1}_{ik}Z^\dagger_{kj}\} = \delta_{mi}\delta_{nj} \tag{30}$$

for $j > i$ and $n > m$. Using the skew symmetry of the matrix Z, we can write a relation which is true for every i, j, m, n

$$\{Z_{mn}, P_{ij}\} = \{Z_{mn}, i(\mathbf{1} + Z^\dagger Z)^{-1}_{ik} Z^\dagger_{kj}\} = \delta_{mi}\delta_{nj} - \delta_{ni}\delta_{mj} \ . \tag{31}$$

From the above relation it is a straightforward but tedious exercise to obtain the Poisson bracket between the components of the matrices Z and $Z^\dagger$

$$\{Z_{mn}, Z^\dagger_{ij}\} = i\big[(\mathbf{1} + Z^\dagger Z)_{mj}(\mathbf{1} + Z^\dagger Z)_{in} - (\mathbf{1} + Z^\dagger Z)_{nj}(\mathbf{1} + Z^\dagger Z)_{im}\big] \ . \tag{32}$$

The components of the matrix Z (or $Z^\dagger$) have zero Poisson bracket with themselves as they are coordinates of the configuration space in the Lagrange formulation.

Therefore, with the Poisson bracket, Eq. (32), we can use the classical Hamiltonian $\mathcal{H}(Z, Z^\dagger)$ (the expectation value of the quantum Hamiltonian of the system for pure states, or the thermal Hamiltonian, Eq. (7), for mixed states) together with the Poisson bracket, Eq. (32), to describe the system. In this way the quantum dynamics is approximated by a classical Hamiltonian dynamics for the parameters of trial states. The Poisson bracket is not in the canonical form, but, due to Darboux theorem, there is a local system of coordinates in which it has the canonical form. Nevertheless, we do not need to find the canonical system of coordinates in practice.

6 Discussion

The variational formalism with the trial states of the form given in Eq. (13) was developed for an arbitrary finite number, N, of fermionic or bosonic operators. We are now at the position to discuss the limit $N \to \infty$, relevant for quantum field theories.

For a field theory (we have in mind the nonrelativistic Schrödinger field theory as the simplest example) there are an infinite number of creation and annihilation operators. The indices i can be taken as the coordinates of the space in which the field theory lives plus the spin indices and the sums will be replaced by integrals. In this way the parameters of the trial state, Eq. (13), become an infinite matrix Z_{x_1,x_2} which is a complex two-point function. Therefore, the finite number of creation/annihilation operators case can be generalized to a classical Hamiltonian field theory for the complex function $Z(x_1, x_2)$. The classical Hamiltonian will be obviously the expectation value of the quantum Hamiltonian on the trial states, but the Poisson bracket will be highly non-trivial being non-local. It is of interest to see how to apply further approximations to this non-local Poisson bracket. This subject is under investigation.

The formalism presented is general. To have a taste of its power we collect below some results obtained in one of the simplest imaginable case, namely

the one-dimensional quantum system [18]. For this case we have the bosonic creation and annihilation operators, a, $a^\dagger$, we restrict ourselves to pure state, and, slightly generalizing the trial state, Eq. (13), we use the following trial state

$$|Z\eta\rangle = \mathrm{e}^{\frac{1}{2}Za^\dagger a^\dagger + \eta a^\dagger}\,|0\rangle\ , \tag{33}$$

where Z and η are two complex parameters. The above trial state is a Gaussian and the parameter η is related to its mean position and the parameter Z to its width. One can obtain, using simple but long algebraic manipulations as above, the following expectations values:

$$\frac{\langle Z\eta|\, a\,|Z\eta\rangle}{\langle Z\eta|Z\eta\rangle} = \frac{\eta + \eta^* Z}{1 - ZZ^*}\ , \tag{34}$$

$$\frac{\langle Z\eta|\, a\, a\,|Z\eta\rangle}{\langle Z\eta|Z\eta\rangle} = \left(\frac{\eta + \eta^* Z}{1 - ZZ^*}\right)^2 + \frac{Z}{1 - ZZ^*}\ , \tag{35}$$

$$\frac{\langle Z\eta|\, a^\dagger a\,|Z\eta\rangle}{\langle Z\eta|Z\eta\rangle} = \frac{(\eta + \eta^* Z)(\eta^* + \eta Z^*)}{(1 - ZZ^*)^2} + \frac{ZZ^*}{1 - ZZ^*}\ . \tag{36}$$

The expectation value of $a^\dagger$ is the complex conjugate of Eq. (34) and the expectation value of $a^\dagger a^\dagger$ is the complex conjugate of Eq. (35). The norm of the considered trial state is proven to be

$$\ln\langle Z\eta|Z\eta\rangle = -\frac{1}{2}\ln(1 - ZZ^*) + \frac{\eta\eta^*}{1 - ZZ^*} + \frac{1}{2}\frac{\eta^2 Z^* + {\eta^*}^2 Z}{1 - ZZ^*}\ . \tag{37}$$

If we take a Hamiltonian, H, expressed in terms of the operators $a^\dagger$, a, it is only a problem of algebra to calculate $\mathcal{H}(Z, \eta, Z^*, \eta^*)$ as its expectation value on the trial state. The classical dynamics in the space of the complex trial state parameters is given by the Lagrangian

$$\mathcal{L} = \frac{i}{2}\left[\left(\frac{\eta^* + \eta Z^*}{1 - ZZ^*}\right)^2 + \frac{Z^*}{1 - ZZ^*}\right]\frac{dZ}{dt} + i\frac{\eta^* + \eta Z^*}{1 - ZZ^*}\frac{d\eta}{dt} - \mathcal{H}(Z, \eta, Z^*, \eta^*) \tag{38}$$

or, alternatively, by the classical Hamiltonian, $\mathcal{H}(Z, \eta, Z^*, \eta^*)$, with the non-vanishing Poisson brackets

$$\begin{aligned}
\{Z, Z^*\} &= -2i(1 - ZZ^*)^2 \\
\{Z, \eta^*\} &= 2i(\eta^* + \eta Z^*)(1 - ZZ^*) \\
\{\eta, \eta^*\} &= -2i(\eta^* + \eta Z^*)(\eta + \eta^* Z) - i(1 - ZZ^*)
\end{aligned} \tag{39}$$

together with their complex conjugates. In this way the quantum dynamics of the one-dimensional problem is approximated by the classical Hamiltonian dynamics in a two dimensional complex space, or a four dimensional

real space. It is obvious that, despite of its classical character, the dynamics retains some quantum effects through the increased dimensionality of the phase space, and the above Poisson brackets. We want to stress that the above Poisson brackets reduce to the usual Poisson bracket

$$\{\eta, \eta^*\} = -i \,, \tag{40}$$

if we impose the constraints $Z = 0$ and $Z^* = 0$ (they are second class constraints in the terminology of Dirac), as it should be (to impose the constraints it is not enough to put $Z = Z^*$ in the last of Eqs. (39), we need to follow the Dirac prescription).

Alternatively, we can impose the constraints $\eta = \eta^* = 0$. They are also second class constraints and we get

$$\{Z, Z^*\} = -2i(1 - ZZ^*)^2 \,. \tag{41}$$

This corresponds to our initial trial state, Eq. (13), for this simple one-dimensional case (it happens that the above Poisson bracket coincides with the first Eqs. (39)!).

7 Conclusions

We have presented a classical description for the dynamics of the parameters of a trial states. The formalism works in the same way for pure and mixed state descriptions of a system, the only difference being the number of dimensions of the configuration space.

This description can be extended to infinite dimensional quantum system where it results into a classical field theory for the parameters of the trial state; the fields are two-point complex functions and further approximations might be introduced in the same way as in the Green functions formalism as the one-particle Green functions are also two-point functions. The difference is that the formalism is completely deterministic and there are no problems with the nonlocality in time of some of the quantities involved.

The present description includes some quantum effects despite the fact that the equation of motion looks classically. It could be an alternative to the nonequilibrium Green function formalism for description of time evolution of systems with important quantum effects, as is the case for heavy ion collisions, especially in the initial stage.

The methods developed in this work were particularized to the simple case of a one-dimensional quantum system. The Lagrangian and the Poisson brackets for the Hamiltonian formalism has been given.

The present approach can be used to treat a system of bosons, or a coupled fermion-boson system, as quantum hadrodynamics [17] which is the modern way for describing the nuclear many-body problem in the framework of effective field theories.

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