Path integral approach for many-fermion systems and an extension of the time-dependent Hartree-Fock method

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The quantization of an extended time-dependent Hartree-Fock equation is performed by using the path integral formalism. The path integral form of time evolution operator between initial and final states is obtained with the use of the completeness relation of the fermion coherent states. It is shown that the extended time-dependent Hartree-Fock equation is naturally derived as a classical limit of the path integral.

While the time-dependent Hartree-Fock (TDHF) method is suitable for the microscopic description of large amplitude collective motion,[1] the application of this method has been limited so far only to systems having an equal number of particles and holes; moreover, it is necessary to quantize the equation derived with the TDHF method, because the TDHF equation is the classical equation of motion. Therefore, to treat quantum systems of odd fermion number or different numbers of particles and holes, an extension of the conventional TDHF method is needed. Recently, Yamamura and Kuriyama[2,3] proposed such an extension of the TDHF method, and performed the quantization of the extended TDHF equation by applying Dirac brackets.[4] Then they have pointed out that the result obtained is equivalent to the boson-fermion expansion of many fermion systems formulated by Marshalek.[5] On the other hand, the path integral provides the other possible quantization method.[6,7] Kuratsuji and Suzuki[7] have developed the path integral technique for the quantization of the TDHF equation based on the completeness relation of the generalized coherent states. However, their method is only limited to the quantization of the conventional TDHF equation. In this paper, therefore, we show that the path integral method also provides the quantization of the extended TDHF equation.

In general, any Slater determinant can be written as

$$|Z\rangle = N \exp\left(\sum_{\lambda i} Z_{\lambda i} \hat{a}_\lambda^\dagger \hat{b}_i^\dagger \right) |\phi_0\rangle \quad , \tag{1}$$

where $|\phi_0\rangle$ is a fixed Slater determinant, and N is a normalization factor. $\hat{a}_\lambda^\dagger$ and $\hat{b}_i^\dagger$ are, respectively, the particle and hole operator with respect to $|\phi_0\rangle$. The coefficient $Z_{\lambda i}$ is $m \otimes n$ matrix where m and n denote the number of the particle and hole states, respectively. Hereafter, we use Greek letters for particle states and Latin letters for hole states. The Slater determinant (1) is also written as follows:

$$|Z\rangle = U|\phi_0\rangle \quad , \tag{2}$$

where U is the unitary operator defined by

$$U = \exp\left(\sum_{\lambda i} (\hat{a}_\lambda^\dagger \hat{b}_i^\dagger F_{i\lambda} - F_{i\lambda}^* \hat{b}_i \hat{a}_\lambda) \right) \quad . \tag{3}$$

Using this unitary operator, the particle and hole operators with respect to $|Z\rangle$ are expressed as

$$\begin{aligned} \hat{\xi}_\lambda &= U\hat{a}_\lambda U^{-1} = \sum_\mu \hat{a}_\mu D_{\mu\lambda} - \sum_j \hat{b}_j^\dagger C_{j\lambda} \quad , \\ \hat{\eta}_i &= U\hat{b}_i U^{-1} = \sum_j D_{ij}\hat{b}_j + \sum_\mu C_{i\mu}\hat{a}_\mu^\dagger \quad , \end{aligned} \tag{4}$$

where $D_{\mu\lambda}$, D_{ij}, and $C_{i\lambda}$ are defined as follows:

$$\begin{aligned} D_{\mu\lambda} &= [\cos(F^\dagger F)^{1/2}]_{\mu\lambda} = [(1+Z^\dagger Z)^{-1/2}]_{\mu\lambda} \quad , \\ D_{ij} &= [\cos(FF^\dagger)^{1/2}]_{ij} = [(1+ZZ^\dagger)^{-1/2}]_{ij} \quad , \\ C_{i\lambda} &= [\sin(FF^\dagger)^{1/2}(FF^\dagger)^{-1}F]_{i\lambda} = [(1+ZZ^\dagger)^{-1/2}Z]_{\lambda i} \quad . \end{aligned} \tag{5}$$

The inverse relationships are given as follows:

$$\hat{a}_\lambda = \sum_\mu \hat{\xi}_\mu D_{\mu\lambda} + \sum_j \hat{\eta}_j^\dagger C_{j\lambda} \quad , \tag{6}$$

$$\hat{b}_i = \sum_j D_{ij}\hat{\eta}_j - \sum_\mu C_{i\mu}\hat{\xi}_\mu^\dagger \quad . \tag{7}$$

In order to obtain the classical image of the particles and holes with respect to $|Z\rangle$, we introduce the fermion coherent state:[2,8]

$$|c\rangle = N' \exp\left(\sum_\lambda \hat{\xi}_\lambda^\dagger x_\lambda + \sum_i \hat{\eta}_i^\dagger y_i \right) |Z\rangle \quad , \tag{8}$$

which satisfies $\hat{\xi}_\lambda |c\rangle = x_\lambda |c\rangle$, $\hat{\eta}_i |c\rangle = y_i |c\rangle$. Here N' is a normalization factor, and (x_λ, x_λ^*) and (y_i, y_i^*) are Grassmann numbers which satisfy the following relationships:

$$\begin{aligned} & x_\lambda x_\mu^* = -x_\mu^* x_\lambda, \quad x_\lambda x_\mu = -x_\mu x_\lambda \quad , \\ & x_\lambda \hat{\xi}_\mu^\dagger = -\hat{\xi}_\mu^\dagger x_\lambda, \quad x_\lambda \hat{\xi}_\mu = -\hat{\xi}_\mu x_\lambda \quad , \\ & y_i y_j^* = -y_j^* y_i, \quad y_i y_j = -y_j y_i \quad , \\ & y_i \hat{\eta}_j^\dagger = -\hat{\eta}_j^\dagger y_i, \quad y_i \hat{\eta}_j = -\hat{\eta}_j y_i \quad . \end{aligned} \tag{9}$$

Here, the fermion coherent state $|c\rangle$ satisfies the completeness relation:[9]

$$\int d\mu(c) |c\rangle\langle c| = 1 \quad , \tag{10}$$

where the invariant measure $d\mu(c)$ is given by

$$d\mu(c) \propto [\det(1+ZZ^\dagger)]^{-(m+n)} \prod_{\lambda i} d(\mathrm{Re}Z_{\lambda i})\, d(\mathrm{Im}Z_{\lambda i}) \prod_\lambda dx_\lambda^* dx_\lambda \prod_i dy_i^* dy_i \quad . \tag{11}$$

Next, in order to derive the path integral form of the propagator, we consider the matrix element of the time evolution operator $\exp(-i\hat{H}t)$ between the initial state $|c_i\rangle$ and the final state $|c_f\rangle$:

$$K(c_f,t_f|c_i,t_i)=\langle c_f|\exp[-i\hat{H}(t_f-t_i)/\hbar)]|c_i\rangle \quad . \tag{12}$$

By dividing the operator $\exp[-i\hat{H}(t_f-t_i)]$ into N equal segments [the time interval $\epsilon=(t_f-t_i)/N$], and then by inserting the completeness relation (10), the propagator (12) becomes

$$\begin{aligned} K(c_f,t_f|c_i,t_i)&=\int\cdots\int\prod_{k=1}^{N-1}d\mu(c_k)\left\langle c_k\left|\left(1-\frac{i}{\hbar}\epsilon\hat{H}\right)\right|c_{k-1}\right\rangle \\ &=\int\cdots\int\prod_{k=1}^{N-1}d\mu(c_k)\exp\left[\frac{i}{\hbar}\epsilon\sum_{k=1}^{N}\left(-\frac{i\hbar}{\epsilon}\log\langle c_k|c_{k-1}\rangle-\frac{\langle c_k|\hat{H}|c_{k-1}\rangle}{\langle c_k|c_{k-1}\rangle}\right)\right] \quad , \end{aligned} \tag{13}$$

with $|c_0\rangle=|c_i\rangle$ and $|c_N\rangle=|c_f\rangle$. By defining $|\Delta c_k\rangle=|c_k\rangle-|c_{k-1}\rangle$, the propagator (13) can be written as follows:

$$K(c_f,t_f|c_i,t_i)=\int\cdots\int\prod_{k=1}^{N-1}d\mu(c_k)\exp\left[\frac{i}{\hbar}\epsilon\sum_{k=1}^{N}\left(\frac{i\hbar}{\epsilon}\langle c_k|\Delta c_k\rangle-\langle c_k|\hat{H}|c_k\rangle\right)\right] \quad .$$

In the limit of $N\to\infty$, which correspond to $1/\epsilon|\Delta c_k\rangle\to\partial/\partial t|c_k\rangle$, $\epsilon\to dt$, and $\sum_{k=1}^{N}\to\int_{t_i}^{t_f}$, we obtain the path integral form of the propagator (12) as follows:

$$K(c_f,t_f|c_i,t_i)=\int\prod_t d\mu[c(t)]\exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f}\left\langle c\left|i\hbar\frac{\partial}{\partial t}-\hat{H}\right|c\right\rangle dt\right)=\int D[\mu(c)]\exp\left(\frac{i}{\hbar}S\right) \quad , \tag{14}$$

where

$$D[\mu(c)]=\prod_t d\mu[c(t)],\quad S=\int_{t_i}^{t_f}Ldt \quad , \tag{15}$$

with

$$L=\left\langle c\left|i\hbar\frac{\partial}{\partial t}-\hat{H}\right|c\right\rangle \quad . \tag{16}$$

The first term on the right-hand side (RHS) of the Lagrangian L can be written as

$$i\hbar\left\langle c\left|\frac{\partial}{\partial t}\right|\right\rangle=i\hbar\left[\sum_\lambda\left(\dot{x}_\lambda\left\langle c\left|\frac{\partial}{\partial x_\lambda}\right|c\right\rangle+\dot{x}_\lambda^*\left\langle c\left|\frac{\partial}{\partial x_\lambda^*}\right|c\right\rangle\right)+\sum_i\left(\dot{y}_i\left\langle c\left|\frac{\partial}{\partial y_i}\right|c\right\rangle+\dot{y}_i^*\left\langle c\left|\frac{\partial}{\partial y_i^*}\right|c\right\rangle\right)+\sum_{\lambda i}\left(\dot{Z}_{\lambda i}\left\langle c\left|\frac{\partial}{\partial Z_{\lambda i}}\right|c\right\rangle+\dot{Z}_{\lambda i}^*\left\langle c\left|\frac{\partial}{\partial Z_{\lambda i}^*}\right|c\right\rangle\right)\right] \quad . \tag{17}$$

Here, we notice the following relationships:

$$\begin{aligned} &\left\langle c\left|\frac{\partial}{\partial x_\lambda}\right|c\right\rangle=-\tfrac{1}{2}x_\lambda^*,\quad \left\langle c\left|\frac{\partial}{\partial x_\lambda^*}\right|c\right\rangle=-\tfrac{1}{2}x_\lambda,\quad \left\langle c\left|\frac{\partial}{\partial y_i}\right|c\right\rangle=-\tfrac{1}{2}y_i^*,\quad \left\langle c\left|\frac{\partial}{\partial y_i^*}\right|c\right\rangle=-\tfrac{1}{2}y_i \quad , \\ &\left\langle c\left|\frac{\partial}{\partial Z_{\lambda i}}\right|c\right\rangle=\tfrac{1}{2}I_{\lambda i}^*+\tfrac{1}{2}K_{\lambda i}^*,\quad \left\langle c\left|\frac{\partial}{\partial Z_{\lambda i}^*}\right|c\right\rangle=-\tfrac{1}{2}I_{\lambda i}-\tfrac{1}{2}K_{\lambda i} \quad , \end{aligned} \tag{18}$$

where $I_{\lambda i}^*$ and $K_{\lambda i}^*$ are given by

$$\begin{aligned} I_{\lambda i}^*=&\left(\frac{Z^\dagger}{1+ZZ^\dagger}\right)_{\lambda i}+\sum_{\lambda'\mu'}x_{\lambda'}^*x_{\mu'}\left\{\left[D\left(\frac{\partial D}{\partial Z_{\lambda i}}\right)-\left(\frac{\partial D}{\partial Z_{\lambda i}}\right)D\right]+\left[C^\dagger\left(\frac{\partial C}{\partial Z_{\lambda i}}\right)-\left(\frac{\partial C^\dagger}{\partial Z_{\lambda i}}\right)C\right]\right\}_{\mu'\lambda'} \\ &-\sum_{i'j'}y_{i'}^*y_{j'}\left\{\left[D^T\left(\frac{\partial D^T}{\partial Z_{\lambda i}}\right)-\left(\frac{\partial D^T}{\partial Z_{\lambda i}}\right)D^T\right]+\left[C^*\left(\frac{\partial C^T}{\partial Z_{\lambda i}}\right)-\left(\frac{\partial C^*}{\partial Z_{\lambda i}}\right)C^T\right]\right\}_{j'i'} \quad , \\ K_{\lambda i}^*=&\sum_{\lambda'j'}y_{j'}x_{\lambda'}\left\{\left[D\left(\frac{\partial C^\dagger}{\partial Z_{\lambda i}}\right)+\left(\frac{\partial c^\dagger}{\partial Z_{\lambda i}}\right)D\right]-\left[C^\dagger\left(\frac{\partial D}{\partial Z_{\lambda i}}\right)+\left(\frac{\partial D}{\partial Z_{\lambda i}}\right)C^\dagger\right]\right\}_{\lambda'j'} \\ &+\sum_{\lambda'j'}x_{\lambda'}^*y_{j'}^*\left\{\left[D\left(\frac{\partial C}{\partial Z_{\lambda i}}\right)+\left(\frac{\partial C}{\partial Z_{\lambda i}}\right)D\right]-\left[C\left(\frac{\partial D}{\partial Z_{\lambda i}}\right)+\left(\frac{\partial D}{\partial Z_{\lambda i}}\right)C\right]\right\}_{j'\lambda'} \quad . \end{aligned} \tag{19}$$

With the use of the Eqs. (17) and (18), the Lagrangian L is rewritten as

$$L=\frac{1}{2}i\hbar\left(\sum_{\lambda}(x_\lambda^*\dot{x}_\lambda-\dot{x}_\lambda^*x_\lambda)+\sum_i(y_i^*\dot{y}_i-\dot{y}_i^*y_i)+\sum_{\lambda i}[\dot{Z}_{\lambda i}(I_{\lambda i}^*+K_{\lambda i}^*)-\dot{Z}_{\lambda i}^*(I_{\lambda i}+K_{\lambda i})]\right)-\tilde{H}\ , \quad (20)$$

where

$$\tilde{H}=\langle c|\hat{H}|c\rangle\ . \quad (21)$$

Note that, since we introduce $C_{\lambda i}$ and $C_{\lambda i}^*$, there occurs a double counting problem of degrees of freedom. Here, in order to avoid this difficulty, we introduce the following constraints:[2]

$$K_{\lambda i}=0,\ \ K_{\lambda i}^*=0\ . \quad (22)$$

Now we examine the classical limit of the propagator (14) under the constraints (22).[10] The classical propagator is obtained with the stationary phase approximation:

$$K^{\rm cl}\sim\exp(iS^{\rm cl}/\hbar)\ . \quad (23)$$

Here the classical action $S^{\rm cl}$ satisfies the variational equation $\delta S=0$ under the constraints (22), and then the classical equations of motion are obtained as follows:

$$\sum_{\lambda' i'}\dot{Z}_{\lambda' i'}\frac{\partial I_{\lambda' i'}^*}{\partial Z_{\lambda i}^*}=-\frac{i}{\hbar}\frac{\partial \tilde{H}'}{\partial Z_{\lambda i}^*}\ ,$$

$$\sum_{\lambda' i'}\dot{Z}_{\lambda' i'}^*\frac{\partial I_{\lambda' i'}}{\partial Z_{\lambda i}}=\frac{i}{\hbar}\frac{\partial \tilde{H}'}{\partial Z_{\lambda i}}\ , \quad (24a)$$

$$i\hbar\dot{x}_\lambda=\{x_\lambda,\tilde{H}\}_D-i\hbar\sum_{\lambda' i'}\left(\frac{\partial I_{\lambda' i'}^*}{\partial x_\lambda^*}\dot{Z}_{\lambda' i'}-\dot{Z}_{\lambda' i'}^*\frac{\partial I_{\lambda' i'}}{\partial x_\lambda^*}\right)\ , \quad (24b)$$

$$i\hbar\dot{x}_\lambda^*=\{x_\lambda^*,\tilde{H}\}_D+i\hbar\sum_{\lambda' i'}\left(\frac{\partial I_{\lambda' i'}^*}{\partial x_\lambda}\dot{Z}_{\lambda' i'}-\dot{Z}_{\lambda' i'}^*\frac{\partial I_{\lambda' i'}}{\partial x_\lambda}\right)\ , \quad (24c)$$

$$i\hbar\dot{y}_i=\{y_i,\tilde{H}\}_D-i\hbar\sum_{\lambda' i'}\left(\frac{\partial I_{\lambda' i'}^*}{\partial y_i^*}\dot{Z}_{\lambda' i'}-\dot{Z}_{\lambda' i'}^*\frac{\partial I_{\lambda' i'}}{\partial y_i^*}\right)\ , \quad (24d)$$

$$i\hbar\dot{y}_i^*=\{y_i^*,\tilde{H}\}_D+i\hbar\sum_{\lambda' i'}\left(\frac{\partial I_{\lambda' i'}^*}{\partial y_i}\dot{Z}_{\lambda' i'}-\dot{Z}_{\lambda' i'}^*\frac{\partial I_{\lambda' i'}}{\partial y_i}\right)\ , \quad (24e)$$

where $\tilde{H}'$ denotes $\tilde{H}$ under the constraints (22). Here, the Dirac bracket[4] is given by

$$\{A,B\}_D=\{A,B\}-\sum_{\alpha\beta}\{A,\phi_\alpha\}\{\phi_\alpha,\phi_\beta\}^{-1}\{\phi_\beta,B\}\ , \quad (25)$$

where ϕ_α is defined for $\alpha=(\lambda i)$ by

$$\phi_\alpha=\begin{cases}K_\alpha, & \alpha=1,2,3,\ldots,nm\ ,\\ K_{\alpha-nm}^*, & \alpha=1+nm,2+nm,\ldots,2nm\ ,\end{cases} \quad (26)$$

and the symbol { } denotes the modified Poisson bracket[9] including the Grassmann variables. Equations (24) are essentially the same equations as those obtained by Kuriyama and Yamamura.[3] If the degrees of freedom x_λ, x_λ^*, y_i, and y_i^* are frozen in Eqs. (24), the classical equations of motion (24) can be reduced as follows:

$$\dot{Z}^\dagger=\frac{i}{\hbar}\left[(1+Z^\dagger Z)\left(\frac{\partial\tilde{H}'}{\partial Z}\right)(1+ZZ^\dagger)\right]\ ,$$

$$\dot{Z}=-\frac{i}{\hbar}\left[(1+ZZ^\dagger)\left(\frac{\partial\tilde{H}'}{\partial Z}\right)(1+Z^\dagger Z)\right]\ . \quad (27)$$

This is just the TDHF equation derived by Kuratsuji and Suzuki.[7] Therefore, Eqs. (24) are considered to be an extension of the TDHF equation including the Grassmann variables.

While the path integral method is identical to the perturbative expansion method, its application is not restricted to the perturbative system. Therefore, for the large amplitude collective phenomena in which the nonlinearity in classical equations (24) becomes large, the path integral method is considered to provide a more useful device comparing the conventional perturbative approach.

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