Semiclassical quantization of the extended time-dependent Hartree-Fock equation: Schematic two-level model

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A semiclassical method of evaluating the path integral over collective (Bose) and independent-particle (Fermi) fields is represented. As an illustration, the schematic two-level model is adopted. The semiclassical calculation of the energy spectra is performed and the result obtained is compared with the exact one.

The time-dependent Hartree-Fock (TDHF) method provides an intuitive understanding of various collective phenomena in many-fermion systems.[1] In the development of this method, however, there are two main problems: one is how to extract the collective subspace from whole fermion Hilbert space, and the other is how to quantize the TDHF equation, because the TDHF equation is the classical equation. For these problems, Yamamura and Kuriyama recently proposed an extended TDHF method[2] which deals with not only collective motion but also independent-particle motion, and the quantization of the extended TDHF equation was performed[3] by applying Dirac brackets.[4,5] On the other hand, the author has recently proposed the other possible quantization method[6] of the extended TDHF equation by using the fermion coherent state path integral. The exact evaluation of the functional integral is, however, rather difficult because of the nonlinear structure of the extended TDHF equation. The purpose of this paper is to investigate the approximate quantization of the extended TDHF equation, and to obtain the approximate energy spectra of the bound states of many-fermion systems. For this aim, we use the semiclassical quantization method of Dashen, Hasslacher, and Neueu[7] who show how the WKB approximation is derived by using the path integral. Their work was based on the ideas developed by Gutwiller, Maslov, and Keller.[8] The quantization rule,[9] analogous to the Bohr-Sommerfeld quantization rule, can be obtained by applying a stationary phase approximation on the path integral. We adopt the schematic two-level model as an illustration in this paper, and show that the present method reproduce fairly well the exact energy spectra.

Let us consider the following schematic Hamiltonian of the two-level system with the same spin j:

$$\hat{H}=\epsilon\hat{J}_z-V(\hat{J}_+\hat{J}_-+\hat{J}_-\hat{J}_+)\ ,$$
$$\hat{J}_+=\sum_m \hat{a}_m^\dagger\hat{b}_m^\dagger,\quad \hat{J}_-=(\hat{J}_+)^\dagger\ , \tag{1}$$

$$\hat{J}_z=\tfrac{1}{2}(\hat{N}-\Omega)=\tfrac{1}{2}\left[\sum_m(a_m^\dagger\hat{a}_m+\hat{b}_m^\dagger\hat{b}_m)-\Omega\right]\ , \tag{2}$$

with $\Omega=j+\frac{1}{2}$. The operators $\hat{a}_m^\dagger$ and $\hat{b}_m^\dagger$ create the particle in the upper level and the hole in the lower level, respectively. The quasispin operators satisfy the algebra of SU(2):

$$[\hat{J}_+,\hat{J}_-]=2\hat{J}_z,\quad [\hat{J}_z,\hat{J}_\pm]=\pm\hat{J}_\pm\ . \tag{3}$$

The generalized coherent state is written as

$$|\zeta\rangle=U|0\rangle=(1+\zeta^*\zeta)^{-\Omega}\exp(\zeta\hat{J}_+)|0\rangle\ , \tag{4}$$

where U is an unitary operator defined by

$$U=\exp(\mu\hat{J}_+-\mu^*\hat{J}_-)\ ,$$

and $|0\rangle$ denotes the particle-hole vacuum, i.e., $\hat{a}_m|0\rangle=\hat{b}_m|0\rangle=0$. By using this unitary operator, the particle and hole operators, with respect to $|\zeta\rangle$, are expressed as

$$\hat{\xi}_m=U\hat{a}_mU^\dagger=(1+\zeta^*\zeta)^{-1/2}\hat{a}_m-(1+\zeta^*\zeta)^{-1/2}\zeta\hat{b}_m^\dagger\ ,$$
$$\hat{\eta}_m=U\hat{b}_mU^\dagger=(1+\zeta^*\zeta)^{-1/2}\hat{b}_m-(1+\zeta^*\zeta)^{-1/2}\zeta\hat{a}_m^\dagger\ . \tag{5}$$

In order to obtain the classical image of the $\hat{\xi}_m$ and $\hat{\eta}_m$, we introduce the fermion coherent state[2,3]

$$|c\rangle=\exp\left[\sum_m(\hat{\xi}_m^\dagger x_m-x_m^*\hat{\xi}_m)+\sum_m(\hat{\eta}_m^\dagger y_m-y_m^*\eta_m)\right]|\zeta\rangle\ . \tag{6}$$

where (x_m,x_m^*) and (y_m,y_m^*) are Grassmann numbers which satisfy the following relationships:

$$x_mx_{m'}^*=-x_{m'}^*x_m,\quad x_mx_{m'}=-x_{m'}x_m\ ,$$
$$x_m\hat{\xi}_{m'}^\dagger=-\hat{\xi}_{m'}^\dagger x_m,\quad x_m\hat{\xi}_{m'}=-\hat{\xi}_{m'}x_m\ ,$$
$$y_my_{m'}^*=-y_{m'}^*y_m,\quad y_my_{m'}=-y_{m'}y_m\ ,$$
$$y_m\eta_{m'}^\dagger=-\eta_{m'}^\dagger y_m,\quad y_m\eta_{m'}=-\eta_{m'}y_m\ . \tag{7}$$

The fermion coherent state (6) satisfies the completeness relation

$$\int d\mu(c)|c\rangle\langle c|=1\ , \tag{8}$$

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

$$d\mu(c)=\frac{2\Omega+1}{\pi(1+\zeta^*\zeta)^2}d(\mathrm{Re}\zeta)d(\mathrm{Im}\zeta)\prod_m dx_m^*dx_m\prod_m dy_m^*dy_m\ . \tag{9}$$

Following the standard procedure[4] of the path integral with the use of completeness relation (8), we obtain the path integral form[6] of the time evolution operator $\exp(-i\hat{H}t/\hbar)$ between the initial state $|c_i\rangle$ and final state $|c_f\rangle$:

$$K(c_f,t_f|c_i,t_i)=\langle c_f|\exp[-i\hat{H}(t_f-t_i)/\hbar]|c_i\rangle$$
$$=\int D[\mu(c)]\exp(iS/\hbar)\ , \tag{10}$$

where

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

with

$$L=\langle c(t)|i\hbar\frac{\partial}{\partial t}-\hat{H}|c(t)\rangle \quad . \tag{11}$$

The Lagrangian L is explicitly written as

$$L=\tfrac{1}{2}i\hbar\left[\sum_m(x_m^*\dot{x}_m-\dot{x}_m^*x_m)+\sum_m(y_m^*\dot{y}_m-\dot{y}_m^*y_m)\right]+i\hbar\frac{\dot{\zeta}}{2(1+\zeta^*\zeta)}\left[\zeta^*\sum_m(1-x_m^*x_m-y_m^*y_m)-2\sum_m(y_mx_m+x_m^*y_m^*)\right]$$
$$-i\hbar\frac{\dot{\zeta}^*}{2(1+\zeta^*\zeta)}\left[\zeta\sum_m(1-x_m^*x_m-y_m^*y_m)-2\sum_m(y_mx_m+x_m^*y_m^*)\right]-H \quad , \tag{12}$$

where the Hamiltonian H is

$$H=\langle c|\hat{H}|c\rangle$$
$$=\epsilon\left[-\frac{1-\zeta^*\zeta}{2(1+\zeta^*\zeta)}\sum_m(1-x_m^*x_m-y_m^*y_m)+\frac{1}{1+\zeta^*\zeta}\sum_m(\zeta^*y_mx_m+\zeta x_m^*y_m^*)\right]$$
$$-\frac{2V}{(1+\zeta^*\zeta)^2}\left[\zeta^*\sum_m(1-x_m^*x_m-y_m^*y_m)+\sum_m(x_m^*y_m^*-\zeta^{*2}y_mx_m)\right]\left[\zeta\sum_m(1-x_m^*x_m-y_m^*y_m)+\sum_m(y_mx_m-\zeta^2x_m^*y_m^*)\right] \quad . \tag{13}$$

Since we introduce the variables ζ and ζ^*, there occurs a double counting problem of degrees of freedom. However, this difficulty can be avoided by introducing the constraints as follows:[2,3,6]

$$\sum_m y_mx_m=\sum_m x_m^*y_m^*=0 \quad . \tag{14}$$

The domain effect of the propagator (10) comes from a path in which the action is stationary $\delta S=0$ under the constraints (14). The variational equation leads to the following equations:

$$\dot{\theta}=0 \quad , \tag{15a}$$

$$\dot{\psi}=2\frac{\epsilon}{\hbar}-\frac{4V}{\hbar}\cos\theta\sum_m(1-x_m^*x_m-y_m^*y_m) \quad , \tag{15b}$$

$$i\hbar\dot{x}_m=A\ x_m,\quad -i\hbar\dot{x}_m^*=A\ x_m^* \quad , \tag{15c}$$

$$i\hbar\dot{y}_m=A\ y_m,\quad -i\hbar\dot{y}_m^*=A\ y_m^* \quad , \tag{15d}$$

with

$$A=(1-\tfrac{1}{2}\cos\theta)\epsilon+V(1-\cos\theta)^2\sum_m(1-x_m^*x_m-y_m^*y_m) \quad ,$$

where we used the other parameters θ and ψ instead of ζ and ζ^* through $\zeta=\tan(\theta/2)\exp(-i\psi)$. These equations are just the extended TDHF equations.[2] Therefore we can say that the present path integral (10) naturally involves the extended TDHF equations (15) as a classical limit.

Now we consider Green's function in the energy representation

$$K(E)=i\int_0^\infty\exp(iET/\hbar)K(T)dT \quad , \tag{16}$$

where $K(T)$ is the trace of the time evolution operator

$$K(T)=\mathrm{Tr}[\exp(-i\hat{H}T/\hbar)]$$
$$=\int d\mu(c_0)\langle c_0|\exp(-i\hat{H}T/\hbar)|c_0\rangle \quad .$$

By using the propagator (10), the Green's function $K(T)$ is expressed as

$$K(T)=\int\bar{D}[\mu(c)]\exp(iS/\hbar) \quad ,$$
$$\bar{D}[\mu(c)]=d\mu(c_0)D[\mu(c)] \quad , \tag{17}$$

where c_0 denotes the end point of the path. By utilizing the stationary phase approximation (SPA) about ζ and ζ^*, we obtain the classical propagator as follows:

$$K^{c1}(T)\propto\int\bar{D}[\mu(x,y)]\exp(iS_\zeta^{c1}/\hbar) \quad , \tag{18}$$

where the notation $\bar{D}[\mu(x,y)]$ represents the Grassmann functional integral. Here the variational principle $\delta_\zeta S=0$ leads to the equations of motion (15a) and (15b). The solutions of equations (15a) and (15b) are $\theta=\alpha$(const) and $\psi=\psi_0-\omega t$ with

$$\omega=2\epsilon/\hbar-4V/\hbar\sum_m(1-x_m^*x_m-y_m^*y_m)\cos\alpha \quad .$$

Then $K^{c1}(T)$ is explicitly written as

$$K^{c1}(T)=\int\bar{D}[\mu(x,y)]\exp\left\{\frac{i}{\hbar}\int_0^T\left[i\hbar\sum_m(x_m^*\dot{x}_m+y_m^*\dot{y}_m)+\frac{\hbar}{2}(1-\cos\alpha)\omega\sum_m(1-x_m^*x_m-y_m^*y_m)\right.\right.$$
$$\left.\left.+\frac{\epsilon}{2}\cos\alpha\sum_m(1-x_m^*x_m-y_m^*y_m)+\frac{V}{2}(1-\cos^2\alpha)\left[\sum_m(1-x_m^*x_m-y_m^*y_m)\right]^2\right]dt\right\} \quad , \tag{19}$$

where we used the relations $d/dt(x_m^*x_m)=d/dt(y_m^*y_m)=0$. If we introduce the functional Gaussian integral

$$\int d[\sigma]\exp\left[-i/\hbar\int_0^T\tfrac{1}{2}\{\sigma+[V(1-\cos^2\alpha)]^{1/2}(1-x_m^*x_m-y_m^*y_m)\}^2\right]dt=\text{const} \quad , \tag{20}$$

the functional integral (19) is written as

$$K^{c1}(T) \propto \exp(iS_0^{c1}) \int \bar{D}[\mu(x,y)]d[\sigma]\exp\left\{\frac{i}{\hbar}\int_0^T \left[i\hbar\sum_m (x_m^*\dot{x}_m + y_m^*\dot{y}_m) - \left\{\frac{\hbar}{2}(1-\cos\alpha)\omega + \frac{\epsilon}{2}\cos\alpha + 2V\Omega(1-\cos^2\alpha) + [V(1-\cos^2\alpha)]^{1/2}\right\}\sum_m (x_m^* x_m + y_m^* y_m) - \frac{\sigma^2}{2}\right]dt\right\} , \tag{21}$$

where

$$S_0^{c1} = \hbar\Omega(1-\cos\alpha)\omega + \epsilon\Omega\cos\alpha + 2\Omega^2 V(1-\cos^2\alpha) .$$

After the integration with the Grassmann variables, the propagator (21) becomes

$$K^{c1}(T) \propto \exp(iS_0^{c1}/\hbar)\sum_n \frac{(2\Omega)!}{(2\Omega-n)!n!}\int d[\sigma]\exp\left\{\frac{i}{\hbar}\int_0^T\left[-\frac{\sigma^2}{2} - \left\{\frac{\hbar}{2}(1-\cos\alpha)\omega + \frac{\epsilon}{2}\cos\alpha + 2\Omega V(1-\cos^2\alpha) + V(1-\cos^2\alpha)\sigma\right\}n\right]dt\right\} . \tag{22}$$

Further, by integrating with the variable σ, we obtain the following result:

$$K^{c1}(T) \propto \sum_n \frac{(2\Omega)!}{(2\Omega-n)!n!}\exp\left\{\frac{i}{\hbar}\left[2V(1-\cos^2\alpha)\left(\Omega-\frac{n}{2}\right)^2 + \epsilon\cos\alpha\left(\Omega-\frac{n}{2}\right)\right]T\right\}\exp\left[i(1-\cos\alpha)\left(\Omega-\frac{n}{2}\right)\omega T\right] . \tag{23}$$

Note that since ωT is 2π for one period T, the correct form of the Green's function is given by the multiple cycles of the periodic orbit[8,9]

$$K^{c1}(T) \propto \sum_n \frac{(2\Omega)!}{(2\Omega-n)!n!}\exp\left\{\frac{i}{\hbar}\left[2V(1-\cos^2\alpha)\left(\Omega-\frac{n}{2}\right)^2 + \epsilon\cos\alpha\left(\Omega-\frac{n}{2}\right)\right]T\right\}\sum_m \exp\left[2m\pi i(1-\cos\alpha)\left(\Omega-\frac{n}{2}\right)\right] . \tag{24}$$

Then the propagator (16) turns out to be

$$K^{c1}(E) \propto \sum_n \frac{(2\Omega)!}{(2\Omega-n)!n!}\exp\left[2\pi i(1-\cos\alpha)\left(\Omega-\frac{n}{2}\right)\right] \times\left\{1-\exp\left[2\pi i(1-\cos\alpha)\left(\Omega-\frac{n}{2}\right)\right]\right\}^{-1}\left[E+2V(1-\cos^2\alpha)\left(\Omega-\frac{n}{2}\right)^2+\epsilon\cos\alpha\left(\Omega-\frac{n}{2}\right)\right]^{-1} . \tag{25}$$

Clearly, $K^{c1}(E)$ has poles about

$$\cos\alpha = 1 - \frac{m}{\Omega - n/2} \equiv -\frac{n'}{\Omega-n/2} , \tag{26}$$

$$E = -2V(1-\cos^2\alpha)\left(\Omega-\frac{n}{2}\right)^2 - \epsilon\cos\alpha\left(\Omega-\frac{n}{2}\right) . \tag{27}$$

Equation (26) is just the quantization rule. Using Eq. (26), the energy (27) is written as

$$E = \epsilon n' + 2Vn'^2 - 2V\left(\Omega-\frac{n}{2}\right)^2 . \tag{28}$$

On the other hand, the exact energy of the Hamiltonian (1) is given by

$$E = \epsilon n' + 2Vn'^2 - 2V\left(\Omega-\frac{n}{2}\right)\left(\Omega-\frac{n}{2}+1\right) . \tag{29}$$

From the comparison between (28) and (29), we find the error $2V(\Omega-n/2)$ which is caused by the factorization $\langle\hat{J}_+\rangle\langle\hat{J}_-\rangle$. This is the quantum correction of order $(1/\Omega)$. The approximate energy spectrum (28) becomes accurate for large Ω. Conclusively, the semiclassical approximation of the path integral method reproduces well the exact energy spectrum of the schematic two-level model.

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