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Time-dependent Hartree-Fock dynamics and phase transition in Lipkin-Meshkov-Glick model

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The time-dependent Hartree-Fock solutions of the two-level Lipkin-Meshkov-Glick model are studied by transforming the time-dependent Hartree-Fock equations into Hamilton's canonical form and analyzing the qualitative structure of the Hartree-Fock energy surface in the phase space. It is shown that as the interaction strength increases these time-dependent Hartree-Fock solutions undergo a qualitative change associated with the ground state phase transition previously studied in terms of coherent states. For two-body interactions stronger than the critical value, two types of time-dependent Hartree-Fock solutions (the "librations" and "rotations" in Hamilton's mechanics) exist simultaneously, while for weaker interactions only the rotations persist. It is also shown that the coherent states with the maximum total pseudospin value are determinants, so that time-dependent Hartree-Fock analysis is equivalent to the coherent state method.

[NUCLEAR STRUCTURE Lipkin-Meshkov-Glick model, TDHF, transformation of TDHF equations to Hamilton's canonical form, coherent states, ground state phase transition.]

I. INTRODUCTION

The two-level model of Lipkin, Meshkov, and Glick[1] (LMG) provides a simple but interesting prototype of the many-body problem. The original authors[1] utilized it to test various approximation techniques. More recently, Krieger[2] has presented numerical solutions for the time-dependent Hartree-Fock (TDHF) approximation in this model for a few selected values of the interaction strength. From an altogether different viewpoint, Gilmore and Feng[3] have applied group theoretical coherent state methods to an analysis of its thermodynamical properties and have studied the "ground state phase transition" which occurs at a certain critical value of the interaction strength.

The present work provides a qualitative analysis of the self-consistent time-dependent Hartree-Fock solutions for the LMG model. We show that the coherent state with the maximum total pseudospin value in this model (and for certain generalizations of this model) are in fact single determinants, so that TDHF studies describe precisely the same physics as the coherent state methods. We show also that every TDHF solution so constructed is periodic in time and belongs to one of two qualitatively distinct classes. Finally, it is shown that at the precise value of the interaction strength at which the ground state phase transition occurs, a qualitative alteration occurs in the spectrum of the TDHF solutions.

II. TDHF EQUATIONS

A. Parametric TDHF equation for the LMG model

For the LMG model[1] of an interacting N-particle system, which is defined by the Hamiltonian

$$H=\frac{\epsilon}{2}\sum_{k=1}^{N}\sum_{\sigma=\pm1}\sigma a_{k,\sigma}^{\dagger}a_{k,\sigma}-\frac{V}{2}\sum_{k,k'=1}^{N}\sum_{\sigma=\pm1}a_{k,\sigma}^{\dagger}a_{k',\sigma}^{\dagger}a_{k',-\sigma}a_{k,-\sigma}\,, \qquad (1)$$

we seek TDHF solutions of the form

$$|\Phi(t)\rangle=\prod_{k=1}^{N}c_k^{\dagger}(t)|0\rangle\,, \qquad (2a)$$

where $|0\rangle$ denotes the vacuum and

$$c_k^{\dagger}(t)=\cos\frac{\theta(t)}{2}a_{k,-1}^{\dagger}+e^{-i\phi(t)}\sin\frac{\theta(t)}{2}a_{k,+1}^{\dagger}\,. \qquad (2b)$$

These wave functions depend on time through two real parameters $\theta(t)$ and $\phi(t)$. This parametrization gives a one-to-one correspondence between $c_k^{\dagger}$ and (θ,ϕ) in the intervals $0\leq\theta\leq\pi$ and $0\leq\phi<2\pi$.

Note that the state $|\Phi\rangle$ in (2a), with $c_k^{\dagger}$ defined by (2b), is not the most general determinantal form. One could allow the parameters θ and ϕ to assume distinct values for each single-particle label k and $|\Phi\rangle$ would still be a determinant. For simplicity, we restrict ourselves here to the special situation defined by Eqs. (2a) and (2b).[4]

The TDHF equations of motion are implied by the variational principle (in units, $\hbar=1$),

$$\delta\int dt\left\langle\Phi(t)\left|H-i\frac{\partial}{\partial t}\right|\Phi(t)\right\rangle=0\,, \qquad (3)$$

in the manifold of single determinantal wave functions Φ.[5,6] For the LMG model, this implies the following two simultaneous equations[7] for the parameters $\theta(t)$ and $\phi(t)$

$$\dot{\theta} = -\epsilon\chi \sin\theta \sin 2\phi \,, \tag{4a}$$

$$\dot{\phi} = \epsilon(1 - \chi\cos\theta\cos 2\phi) \,, \tag{4b}$$

where $\chi = (N-1)V/\epsilon$. Since Eqs. (4) are invariant under the transformation $(\theta, \phi, \chi) \to (\theta', \phi', \chi') = (\theta, \phi + \pi/2, -\chi)$, we can restrict our discussions to positive χ values (i.e., to attractive interactions $V > 0$), without loss of generality.

Since TDHF conserves the average energy,[8] any solution of (4) must lie on an equi-energy contour of the energy surface,

$$\langle H \rangle \equiv \langle \Phi(\theta, \phi) | H | \Phi(\theta, \phi) \rangle = -\frac{N\epsilon}{2}\left(\cos\theta + \frac{\chi}{2}\sin^2\theta\cos 2\phi\right) . \tag{5}$$

In fact, when expressed in terms of $\langle H \rangle$, Eqs. (4) can be written as

$$\dot{\theta} = -\left(\frac{N}{2}\sin\theta\right)^{-1}\frac{\partial\langle H \rangle}{\partial\phi} \,, \tag{6a}$$

$$\dot{\phi} = \left(\frac{N}{2}\sin\theta\right)^{-1}\frac{\partial\langle H \rangle}{\partial\theta} \,, \tag{6b}$$

which are parametric equations for the equi-energy contours of $\langle H \rangle$.

B. TDHF equations in Hamilton's canonical form

Equations (6) can be transformed into Hamilton's canonical form by introducing a coordinate q and its conjugate momentum p, as follows:

$$q = \phi + \pi/4 \,, \tag{7a}$$

$$p = -\frac{N}{2}\cos\theta \,. \tag{7b}$$

The additive constant $\pi/4$ is introduced in (7a) for convenience in displaying the energy surface in this (q, p) (phase) space. Equations (6) then take the canonical form

$$\dot{q} = \frac{\partial\mathcal{K}(q,p)}{\partial p} \,, \tag{8a}$$

$$\dot{p} = -\frac{\partial\mathcal{K}(q,p)}{\partial p} \,, \tag{8b}$$

with the Hamiltonian $\mathcal{K}$ given as a function of q and p by the Hartree-Fock energy (5):

$$\mathcal{K}(q,p) \equiv \langle H \rangle = \epsilon\left[p - \frac{\chi}{N}\left(\frac{N^2}{4} - p^2\right)\sin 2q\right] . \tag{9}$$

From (7b) and the fact that θ is real, the physical region in the phase space is defined by $-N/2 \leq p \leq N/2$ and all q.

The TDHF solutions are now represented by trajectories in this physical region of the phase space, and follow the classical trajectories associated with the Hamiltonian $\mathcal{K}$. These trajectories are the equi-energy contour lines of $\mathcal{K}$. Note that $\mathcal{K}$ contains a term linear in the momentum and a variable inertia (defined by the coefficient of p^2) which can become negative. This differs from the form of Hamiltonian familiar from the motion of point particles in classical mechanics, which is quadratic in the momentum and has a positive definite inertia.

III. TDHF SOLUTIONS AND GROUND STATE PHASE TRANSITION

A. Energy surface

Since the TDHF solutions are determined by the properties of the energy surface $\mathcal{K}(q,p)$, we turn here to the study of the qualitative structure of this energy surface.

First, we note that $\mathcal{K}(q,p)$ is periodic in q with period π. Therefore, in the region $-N/2 \leq p \leq N/2$ and $0 \leq q < 2\pi$, where all distinct system points are included, the energy surface consists of two identical parts which join one another on the line, $q = \pi$.

Next, we consider the stationary points of $\mathcal{K}$, which are given as functions of the interaction strength χ, as

$$(q_{A_n}, p_{A_n}) = [(n + \tfrac{1}{4})\pi, -N/2\chi] \,, \tag{10a}$$

$$(q_{B_n}, p_{B_n}) = [(n + \tfrac{3}{4})\pi, N/2\chi] \,, \tag{10b}$$

$$(q_{C_m}, p_{C_m}) = (q_{A_n} \pm q_s, -N/2) \,, \tag{10c}$$

$$(q_{D_m}, p_{D_m}) = (q_{B_n} \pm q_s, N/2) \,, \tag{10d}$$

where

$$q_s = \tfrac{1}{2}\cos^{-1}(1/\chi) \,, \tag{10e}$$

n is any integer, and

$$m = \tfrac{1}{2}(4n - 1 \pm 1) \tag{10f}$$

defines two indices for each n value, which correspond in (10c), (10d) with the (+/−) signs, respectively. For $\chi > 1$, (q_{A_n}, p_{A_n}) and (q_{B_n}, p_{B_n}) are minimum and maximum points of $\mathcal{K}$, respectively, lying inside the physical region, while (q_{C_n}, p_{C_n}) and (q_{D_n}, p_{D_n}) are saddle points, lying on the boundaries of this region. Therefore, in this case $(\chi > 1)$, the energy surface has two minima, two maxima, and eight saddle points in the portion of the physical region defined by $0 \leq q \leq 2\pi$ (see Fig. 1).

The structure of the energy surface changes qualitatively when χ passes through the critical value, $\chi_c = 1$. Consider the minimum A_1 and its adjacent saddle points C_1 and C_2 in Fig. 1 for $\chi > 1$. As can be seen from (10), all these three points move towards $(q, p) = (\pi/4, -N/2)$ as χ decreases towards $\chi = 1$. When χ decreases to less

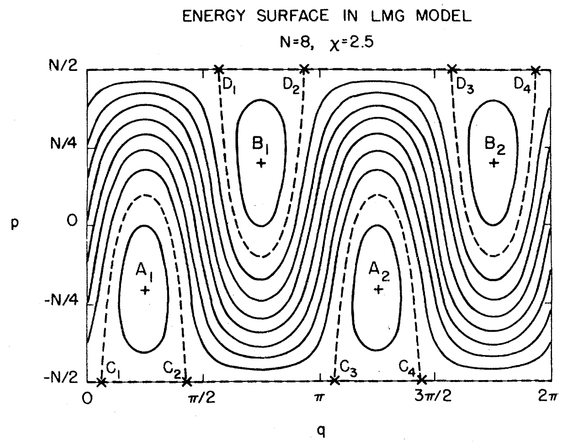

FIG. 1. Contour map of the energy surface $\mathcal{K}(q,p)$ for $N=8$ and $\chi=2.5$. The points A_i and B_i are minima and maxima, respectively, and C_i and D_i are saddle points. Their coordinates are given by Eqs. (10). The contour passing through $(q,p)=(0,0)$ has zero energy. The contours passing through the saddle points are drawn with dashed lines. They separate regions with closed loop contours corresponding to "librations" and region with open curve contours corresponding to "rotations." Successive contours differ in energy by the unperturbed single particle spacing ϵ.

than 1 $(0\leqslant\chi<1)$, A_1 will move into the nonphysical region (where it will become a saddle point), and C_1 and C_2 will move to the imaginary q axis (where they will become minima). For all values of $0\leqslant\chi\leqslant 1$, the points on the straight line $p=-N/2$ have the same energy and are the least energy points within the physical region, although the energy does not have a zero derivative with respect to p at these points. Figure 2 shows an energy surface for $\chi=0.25$.

B. Ground state phase transition

From the discussion in Sec. III A, one sees that the structure of the energy surface undergoes a qualitative change at $\chi=1$. In fact, at this critical value of χ the second derivative of $\mathcal{K}$ with respect to q vanishes at the stationary point $(q_{A_1},p_{A_1})=(\pi/4,-N/2)$.

We define generally a "ground state phase transition" for a stationary Hartree-Fock state by the condition that the minimum of the Hartree-Fock energy surface becomes unstable, as a function of the dimensionless interaction strength parameter χ. More precisely, let (q_0,p_0) be a minimum point of $\mathcal{K}(q,p)$ (or equivalently, $\langle H\rangle$). Then the stationary Hartree-Fock state undergoes a ground state phase transition at $\chi=\chi_0$, if

$$\frac{\partial^2}{\partial q^2}\mathcal{K}(q,p)\bigg|_{(q_0,p_0),\chi_0}=0\,, \tag{11a}$$

or

$$\frac{\partial^2}{\partial p^2}\mathcal{K}(q,p)\bigg|_{(q_0,p_0),\chi_0}=0\,. \tag{11b}$$

Under this definition, the stationary Hartree-Fock solution undergoes a ground state phase transition at $\chi_0=\chi_c=1$.

Conditions (11) are related to the definition of the ground state phase transition given by Gilmore and Feng.[3] They introduce the coherent state defined by

$$\left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle=\exp[-\eta(\Omega)\hat{J}_+ +\eta^*(\Omega)\hat{J}_-]\,|\,\mathrm{ext}\rangle\,. \tag{12}$$

Here $\eta(\Omega)$ is a function of the angles $\Omega\equiv(\theta,\phi)$, $\hat{J}_\pm$ and $\hat{J}_3$ are pseudospin operators[1,3]

$$\hat{J}_+=\hat{J}_-^\dagger=\sum_k a_{k,+1}^\dagger a_{k,-1}\,, \tag{13a}$$

$$\hat{J}_3=\tfrac{1}{2}\sum_{k,\sigma}\sigma\, a_{k,\sigma}^\dagger a_{k,\sigma}\,, \tag{13b}$$

and $|\,\mathrm{ext}\rangle$ is an "extremal" state, which is the state with the lowest (or, equally well, the highest) projection $J_z=-J$ in the subspace with a fixed total pseudospin J. For the subspace with the highest J value, i.e., $J=N/2$, this extremal state is the ground state of the unperturbed Hamiltonian, $H_0=H|_{V=0}$, i.e.,

$$|\,\mathrm{ext}\rangle=|J,-J\rangle=\sum_{k=1}^{N}a_{k,-1}^\dagger|\,0\rangle\,, \tag{14}$$

and is a single Slater determinant.

They then define the "P" and "Q" representations of the Hamiltonian H (not to be confused with canonical coordinates) through the coherent states by

$$H=\frac{2J+1}{4\pi}\int\left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle P_J(H;\Omega)\left\langle\begin{matrix}J\\ \Omega\end{matrix}\right|d\Omega \tag{15a}$$

and

$$Q_J(H;\Omega)=\left\langle\begin{matrix}J\\ \Omega\end{matrix}\right|H\left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle. \tag{15b}$$

These two functions P_J and Q_J of Ω are shown[3] to be the lower and upper bound estimates of the exact ground state energy, respectively, and approach each other as $N\to\infty$. The ground state phase transition (as well as the thermodynamical phase transition) is then inferred by these authors by the loss of the stability for the minima of both P_J and Q_J.

We show in the Appendix that the coherent state $\left|\begin{smallmatrix}J\\ \Omega\end{smallmatrix}\right\rangle$ for $J=N/2$ is identical to the Hartree-Fock state Φ. Therefore, Q_J defined in (15b) for $J=N/2$ is identically the Hartree-Fock energy $\langle H\rangle=\mathcal{K}(q,p)$, and the ground state phase transition for the stationary Hartree-Fock state is related to the ground state phase transition discussed in Ref. 3.

C. TDHF librations and rotations

The qualitative change in the structure of the energy surface gives rise to a qualitative change in the TDHF trajectories. Consider first the situation $\chi > 1$ where we have two minima, two maxima, and eight saddle points in the region $-N/2 \leq p \leq N/2$ and $0 \leq q < 2\pi$ (Fig. 1). The energy surface for such a situation has three types of equi-energy contour curves exhibited in Fig. 1, and hence three types of TDHF trajectories, as follows: (a) closed loops, (b) open curves, and (c) limiting curves (dashed lines) which separate the first two types of curves and which can be regarded as their common limiting curve.

Except for the limiting curves and for loops of zero length (which are just the minimum and maximum points), none of the equi-energy curves pass through any of the stationary points (10). This implies that $\dot{q}$ and $\dot{p}$ can never become zero simultaneously on these curves. Consequently, the time Δt needed to traverse any finite segment of these curves, given by the following integral over the arc length l,

$$\Delta t = \int_{l_0}^{l_1} \frac{dl}{(\dot{q}^2 + \dot{p}^2)^{1/2}}, \tag{16}$$

is finite.

On the other hand, $\dot{q}$ and $\dot{p}$ go to zero at the saddle points through which the limiting curves will pass. In fact, the lowest order terms in the Taylor expansion of the energy surface around any saddle point $(\bar{q},\bar{p})$ [which can be any point given in (10c) and (10d)] are quadratic in $q-\bar{q}$ and $p-\bar{p}$. It follows from this fact and Hamilton's equations (8) that the integrand in Eq. (16) is proportional to l^{-1}, in the neighborhood of a saddle point. This implies a logarithmic divergence at the saddle points for the integral (16). Therefore, the time needed to arrive at any saddle point along a limiting trajectory is infinite.

Thus, for closed loop trajectories (excluding the limiting trajectories) both q and p repeat their values after a specific finite interval of time, and hence they are periodic with a finite period. The motion corresponding to such a closed trajectory is referred to as "libration" in Hamilton's mechanics.[9] Since $\Phi(t)$ depends on t only through p and q, $\Phi(t)$ is also periodic and has the same period as that of p and q. Moreover, because $\mathcal{K}(q,p)$ is identical in the regions $0 \leq q \leq \pi$ and $\pi \leq q \leq 2\pi$, we always have two libration trajectories with identical shape, period, and energy. However, the librational states associated with these trajectories differ by the sign in the last term of (2b) and are, therefore, linearly independent of one another. We conclude that the TDHF librations in the LMG model are doubly degenerate.

The open curves represent another kind of periodic trajectory called "rotation" in Hamilton's mechanics.[9] Here q increases indefinitely, while p repeats itself after a finite period of time. Furthermore, $\Phi(q,p) \equiv \Phi(q+2\pi,p)$, and hence the corresponding wave function $\Phi(t)$ is periodic.[10] And, since there is only one trajectory corresponding to each energy, the rotational states are nondegenerate in the LMG model.

Therefore, for $\chi > 1$ the LMG model simultaneously supports two types of TDHF solutions: the nondegenerate rotations and the doubly degenerate librations.

The situation for $\chi < 1$ is quite different. As already pointed out in Sec. III A, all the stationary points have moved out of the physical region of the phase space. Therefore, there are no closed loop equi-energy contours and hence no closed loop TDHF trajectories (see Fig. 2). We are thus left with only one type of TDHF trajectory, namely, the nondegenerate rotational trajectory.

The transition between these two distinct regions of χ occurs at $\chi_0 = 1$, i.e., at the ground state phase transition. Therefore, we conclude that the TDHF solutions themselves undergo a qualitative change in association with the ground state phase transition. In one region ($0 \leq \chi < 1$), the LMG model gives rise to only one type of TDHF solutions, the nondegenerate rotations, while in the other region ($\chi > 1$), it allows the coexistence of two types of TDHF solutions, the nondegenerate rotations and the doubly degenerate librations.

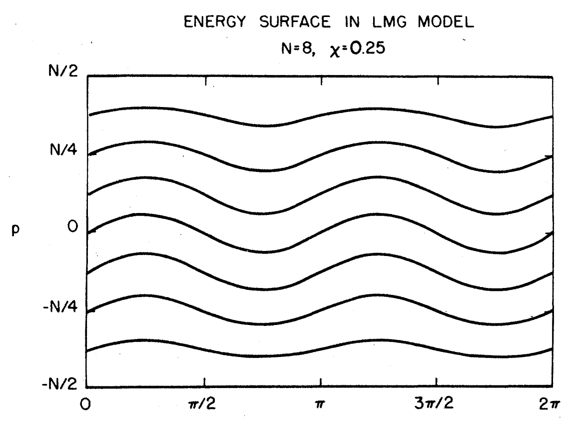

FIG. 2. Contour map of the energy surface $\mathcal{K}(q,p)$ for $N=8$ and $\chi=0.25$. The contour passing through $(q,p) = (0,0)$ has zero energy. The upper and lower boundary line $p = \pm N/2$ are contours of energy $\pm N\epsilon/2$ ($= \pm 4\epsilon$), respectively. Successive contours differ in energy by ϵ.

IV. CONCLUSIONS

By studying the structure of the TDHF energy surface, we have investigated the qualitative behavior of the whole family of TDHF solutions in the LMG model. The TDHF equations of motion are transformed into Hamilton's canonical form. The TDHF solutions are then represented by classical trajectories in a two-dimensional phase space, which trajectories are also the equi-energy contour curves of the TDHF energy surface in this phase space.

The TDHF solutions divide into two distinct qualitative types: (a) those represented by closed loop trajectories (librations), which are doubly degenerate, and (b) those represented by open, but periodic trajectories (rotations), which are nondegenerate.

The minimum of the energy surface becomes unstable at the critical interaction strength $\chi_0=1$ which we define as a ground state phase transition. It is shown that when χ is greater than the critical value $\chi_0=1$, both the librational and rotational TDHF solutions exist simultaneously, and that when χ is smaller than $\chi_0=1$ only the rotational solutions prevail.

Note added. The use of the Lipkin-Meshkov-Glick (LMG) model to illustrate the behavior of systems undergoing a ground state phase transition does not originate in the present work. Besides Refs. 1 to 3, Refs. 11 through 17 and references cited therein should be consulted in order to properly trace the ramification and the evolution of this approach.

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APPENDIX: EQUIVALENCE OF TDHF STATES AND COHERENT STATES

In this appendix, we show that the TDHF determinant defined in (2) is identical to the coherent states with total pseudospin $J=N/2$. This equivalence follows from (a) Thouless's theorem,[18] and (b) the fact that $\hat{J}_+$ and $\hat{J}_-$ in (13) are one-body operators, and (c) that the extremal state in the $J=N/2$ subspace is a Slater determinant. For Thouless's theorem[18] states that any state defined as an exponential function of one-body operators acting on a Slater determinant is also a Slater determinant.

One can also prove this equivalence explicitly by expanding the exponential function in $|{}^{J}_{\Omega}\rangle$ defined by (12) and collecting real and imaginary parts. In this way, one can show that the coherent state $|{}^{J}_{\Omega}\rangle$ is identical to the determinant $|\Phi\rangle$ in (2) at each value of the angles $\Omega=(\theta,\phi)$, i.e.,

$$\left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle \equiv |\Phi\rangle \tag{A1a}$$

with

$$\eta(\Omega)=\frac{\theta}{2}e^{i\phi} \tag{A1b}$$

in Eq. (12). Because of this equivalence the dynamical evolution of the TDHF state is identical with that of the coherent state which satisfied the same variational principle (3).

Note that this equivalence of the coherent state approach and TDHF can be generalized to other models once the conditions for the Thouless theorem are satisfied. In fact, in an extension of the LMG model to multilevel models, Gilmore and Feng[19] have defined the coherent states in exactly the same form as (12) except that each term in the exponent in (12) is replaced by a sum of one-body shift-up or shift-down operators corresponding to different pairs of levels. Therefore, also in these multilevel models, the time evolution of these coherent states which are generated from the extremal state chosen to be unperturbated ground state are identical to the TDHF solutions.

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[4]If the parameters θ and ϕ in (2b) are different for each particle, i.e., if they are replaced by θ_k and ϕ_k, then we shall obtain, instead of the pair of equations (4), N pairs of equations. The right-hand side of each pair will reduce to that of Eqs. (4) if θ_k and ϕ_k for every k are set to equal to θ and ϕ, respectively. It then follows that if one chooses identical initial conditions for all θ_k and ϕ_k they will remain identical, and hence independent of k, for all time. Thus the assumed form (2b) is consistent with the general TDHF dynamical evolution of the system.

[5]Reference 6 shows that this variational principle fixes the time-dependent phase factor of the solution of (3) uniquely. In the present problem, the phase factor is $\exp[i\alpha(t)]$, where

$$\alpha=\int^t \langle\Phi|\, i\partial/\partial t' \,|\,\Phi\rangle dt' - \langle\Phi|\, H \,|\,\Phi\rangle t$$
$$=\int^t \frac{N\epsilon}{2}\left\{1+\frac{\chi}{2}\,[1-\cos\theta(t')]^2\cos 2\phi(t')\right\}dt' .$$

Throughout this paper, this phase factor is replaced by unity [as in Eqs. (2)], since only expectation values, which are independent of this factor, are utilized herein.

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[10]We should emphasize that the "rotations" here describe the motion in the phase (q,p) space constructed from the parametric $\theta\phi$ space, and it has no direct connection with physical rotations in coordinate space.

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