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I. INTRODUCTION

In this paper we use TDHF to study steady state large amplitude nuclear collective motions, such as vibration and rotation. As is well known the small amplitude TDHF leads to the RPA equation. For large amplitudes, recent progress has been made by many people [1-4].

We explore one central aspect of this problem in this paper, namely the periodicity. We consider this aspect to be central because the simplest TDHF description of a collective steady state is a periodic solution. However, the analysis of periodicity in TDHF is not trivial because TDHF is a nonlinear theory and it is not known under what circumstances a nonlinear theory can support periodic solutions. It is also unknown whether such periodic solution, if they exist, form a continuous or a discrete set. But, these properties may be important in obtaining the energy spectrum of the collective states from the TDHF description.

By insisting upon a close analogy with the exact Schroedinger eigenstates, we are led to consider a subset of periodic TDHF solutions, the Gauge Invariant Periodic solutions [5], which are invariant under an arbitrary time-dependent shift in the reference point for measuring the energy.

We investigate the periodicity and Gauge Invariant Periodicity of solutions for that class of models whose TDHF solutions depend on time through two parameters. We find that in such models TDHF supports a continuous family of periodic solutions, but only a discrete subset of

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these is gauge invariant. We further prove that these discrete Gauge Invariant Periodic solutions obey the Bohr-Sommerfeld quantization rule. The energy spectrum of the Gauge Invariant Periodic solutions is compared with the exact eigenenergies in one specific example.

II. GAUGE INVARIANT PERIODIC TDHF SOLUTIONS

Among the periodic solutions, which satisfy

$$\Phi(t+T) \equiv \Phi(t) \quad (2.1)$$

(where T is the period), we consider those which are also gauge invariant. For any TDHF Hamiltonian $\mathcal{H}(t)$, corresponding to the solution $\Phi(t)$, such that

$$\mathcal{H}(t)\Phi(t) = i\hbar \partial\Phi/\partial t, \quad (2.2)$$

we can construct the gauge invariant time evolution operator,

$$\mathcal{H}_G(t) = \mathcal{H}(t) - \langle \mathcal{H}(t) \rangle, \quad (2.3)$$

where $\langle A \rangle \equiv \langle \Phi | A | \Phi \rangle$. This $\mathcal{H}_G$ is manifestly gauge invariant, since any change in the energy reference point effected by the transformation of the exact Hamiltonian H ,

$$H \rightarrow \hat{H} = H + B(t) \quad (2.4)$$

(where $B(t)$ is a c-number), induces exactly the same change in both terms in the right-hand side of (2.3) and hence is cancelled identically.

The Gauge Invariant Periodic TDHF solutions are defined as the solutions Φ_G of $\mathcal{H}_G$, whose complex amplitude is exactly periodic, according to the definition (2.1).

Since $\mathcal{H}_G$ and $\mathcal{H}$ differ only by a time dependent c-number, Φ_G is related to Φ by a phase factor, as follows,

$$\Phi_G(t) = \Phi(t) \exp\left\{i \int_{t_0}^t \langle \mathcal{H}(t') \rangle dt' / \hbar\right\}. \quad (2.5)$$

Therefore, given a periodic solution Φ for a TDHF equation, the corresponding gauge invariant solution will be periodic, if and only if

$$\int_{t_0}^{t_0+T} \langle \mathcal{H} \rangle dt = 2n\pi\hbar, \quad (2.6a)$$

or, by Eq.(2.2),

$$i\hbar \int_{t_0}^{t_0+T} \langle \partial/\partial t \rangle dt = 2n\pi\hbar, \quad (2.6b)$$

where n is an integer.

Since (2.6) is an additional condition imposed upon the periodic solution Φ , not all periodic TDHF solutions will generally be Gauge Invariant Periodic solutions.

Gauge Invariant Periodic Solutions as Analogs of Exact Eigenstates

When this Gauge Invariant Periodic condition (2.6) is satisfied, the corresponding constant- $\langle \mathcal{H} \rangle$ TDHF solution [5,6] Φ_C has the form

$$\begin{aligned} \Phi_C(t) &= \Phi(t) \exp\left\{i \int_{t_0}^t \langle \mathcal{H} \rangle dt' / \hbar - i \langle H \rangle t / \hbar\right\} \\ &= \Phi_C(t) \exp(-i \langle H \rangle t / \hbar) \\ &= (\text{periodic function}) \cdot \exp(-i \langle H \rangle t / \hbar), \end{aligned} \quad (2.7)$$

in close analogy with the exact time-dependent Schroedinger state $\Psi(t)$ corresponding to a given eigenfunction,

$$\Psi(t) = (\text{stationary function}) \cdot \exp(-iEt/\hbar). \quad (2.8)$$

Note that under an arbitrary gauge transformation (2.4), Eqs. (2.7) and (2.8) transform in precisely the same way:

$$\Phi_C(t) \rightarrow \hat{\Phi}_C(t) = \Phi_C(t) \exp(-i \int B(t') dt' / \hbar) \quad (2.9a)$$

$$\Psi(t) \rightarrow \hat{\Psi}(t) = \Psi(t) \exp(-i \int B(t') dt' / \hbar). \quad (2.9b)$$

Eq. (2.7) also implies [5] that when two Gauge Invariant Periodic TDHF solutions are non-degenerate[†], the corresponding constant- $\langle \mathcal{H} \rangle$ solutions

[†]Here degenerate solutions have equal energies, or energies differing by $2n\pi/T$ (n integer) and equal period.

$\phi_C(t)$ are orthogonal in the following time averaged sense:

$$\lim_{\tau \rightarrow \infty} (2\tau)^{-1} \int_{t_0 - \tau}^{t_0 + \tau} \langle \phi_1(t) | \phi_2(t) \rangle dt = 0. \quad (2.10)$$

III. TWO-PARAMETER TDHF MODELS

We study the Gauge Invariant Periodic solutions for a class of models whose TDHF solutions depend on time only through two parameters $\alpha(t)$ and $\beta(t)$. The variational principle,

$$\delta \int dt \langle \phi(\alpha, \beta) | H - i\hbar \partial / \partial t | \phi(\alpha, \beta) \rangle = 0, \quad (3.1)$$

leads to a TDHF equation in the form of two simultaneous equations of motion for the two time-dependent parameters, as follows

$$\dot{\alpha} = \frac{1}{B_{\alpha\beta}} \frac{\partial \langle H \rangle}{\partial \beta} \quad (3.2a)$$

$$\dot{\beta} = - \frac{1}{B_{\alpha\beta}} \frac{\partial \langle H \rangle}{\partial \alpha}. \quad (3.2b)$$

Here, $B_{\alpha\beta}$ is defined by

$$B_{\alpha\beta} = -i\hbar [\langle \phi_\alpha | \dot{\phi}_\beta \rangle - \langle \phi_\beta | \dot{\phi}_\alpha \rangle], \quad (3.3)$$

and the subscripts denote derivatives, so that $\phi_\alpha = \partial \phi / \partial \alpha$, for example.

Any Two-Parameter Model Has a Continuous Set of Periodic TDHF Solutions

From Eq. (3.2) an important conclusion about the periodicity of TDHF solutions can be drawn as follows. Any TDHF solution of the two-parameter model is completely specified by a trajectory in the $\alpha\beta$ parametric space. But the TDHF equation (3.2) implies that such a trajectory is also a constant energy contour of $\langle H \rangle$. Then from the fact that Eqs. (3.2) are first order, it implies that the TDHF solution corresponding to any closed loop contour of $\langle H \rangle$ will be periodic.

On the other hand, for a model which has a stable stationary HF solution, $\langle H \rangle$ has a local minimum at the parameter values of that state. Then, by the continuity of $\langle H \rangle$, this energy surface always possesses a continuous family of closed constant-energy contours in the neighborhood of this mini-

mum, no matter how small this neighborhood. Therefore, for a two-parameter model which has a stable stationary HF solution, there always exists at least one continuous set of periodic TDHF solutions.

TDHF Equation in Canonical Hamiltonian Form

To transform Eq. (3.2) to canonical form, we define a pair of new parameters p and q by the conditions,

$$i\hbar \langle \Phi | \Phi_q \rangle = p \quad (3.4a)$$

$$\langle \Phi | \Phi_p \rangle = 0. \quad (3.4b)$$

One can verify by the chain rule of differentiation that p and q can be obtained from α and β through a transformation $p=p(\alpha, \beta)$ and $q=q(\alpha, \beta)$, which satisfy the differential equations

$$p \frac{\partial q}{\partial \alpha} = i\hbar \langle \Phi | \Phi_\alpha \rangle \quad (3.5a)$$

$$p \frac{\partial q}{\partial \beta} = i\hbar \langle \Phi | \Phi_\beta \rangle. \quad (3.5b)$$

Note that the right-hand side in Eqs. (3.5) is real by virtue of the norm conservation of Φ . We shall prove in the appendix that this pair of differential equations always possesses a solution.

Now, from Eqs. (3.3) and (3.4), we have

$$B_{qp} = 1. \quad (3.6)$$

Hence, the equation of motion (3.2) can be written as

$$\dot{q} = \frac{\partial \mathcal{K}(q, p)}{\partial p} \quad (3.7a)$$

$$\dot{p} = - \frac{\partial \mathcal{K}(q, p)}{\partial q}, \quad (3.7b)$$

with

$$\mathcal{K}(q, p) = \langle H \rangle. \quad (3.8)$$

Eqs. (3.7) are of the canonical Hamiltonian form, with $\mathcal{K}$ playing the role of the Hamiltonian, and q and p as the conjugate coordinate and momentum, respectively. Since α and β are arbitrary, we conclude that any two-parameter

meter TDHF model can be transformed to the canonical form.[†]

Equivalence of Gauge Invariant Periodicity and Bohr-Sommerfeld Quantization

In terms of these canonical variables we can demonstrate the remarkable result that the Gauge Invariant Periodic condition (2.6) is equivalent to the Bohr-Sommerfeld quantization of this two-parameter model. This can be seen by calculating the integrand in Eq. (2.6b) directly:

$$\begin{aligned} i\hbar \langle \Phi | \partial / \partial t | \Phi \rangle &= i\hbar [\dot{q} \langle \Phi | \phi_q \rangle + \dot{p} \langle \Phi | \phi_p \rangle] \\ &= \dot{p} \dot{q}. \end{aligned} \quad (3.9)$$

Then for the periodic solutions where the TDHF trajectory in the qp- (phase) space form a closed loop, the Gauge Invariant Periodic condition (2.6) can be written as

$$\oint \dot{p} \dot{q} = 2n\pi\hbar, \quad (3.10)$$

which is exactly the Bohr-Sommerfeld quantization rule.

Equation (3.10) implies that only those closed loop contours of $\mathcal{K}$ which enclose an area in the phase space equal to an integral multiple of $2\pi\hbar$ are Gauge Invariant Periodic. Hence, the Gauge Invariant Periodic condition selects from the continuous set of periodic TDHF solutions not simply any discrete subset of states, but that particular subset which would have been selected by imposing the Bohr-Sommerfeld quantization rule upon the "classical" trajectories of the TDHF solutions.

IV. AN EXAMPLE

Explicit examples of the two-parameter TDHF model can be constructed using the general formulation discussed in Sect. III. We summarize the results for one example here, the one-dimensional system of two fermions interacting with a harmonic oscillator potential. A more detailed discus-

[†]Some particular examples of this general result are exhibited by Kerman and Koonin [7], where the parametric TDHF problem for arbitrary number of parameters is also discussed.

sion will be published elsewhere [8]. (In addition another example, the Lipkin-Meshkov-Glick model is analyzed in references [8] and [9].)

In this two-fermion system we consider the TDHF solutions corresponding to the monopole vibration of the system. For such a case we need two parameters because the monopole vibration can be specified by the system's overall width and average current at each instant of time.

Using the formulation of Sect. III, we solve the TDHF equation, obtaining solutions which are all periodic. The width of the system $D(t)$ is found to be

$$D(t) = D_e \left[\frac{1}{2} \left(\mu + \frac{1}{\mu} \right) + \frac{1}{2} \left(\mu - \frac{1}{\mu} \right) \cos 2\omega t \right]^{1/2}. \quad (4.1)$$

Here $\mu = (D_0/D_e)^2$, $D_0 = D(0)$, $D_e = \hbar/m\omega$ is the width at equilibrium (i.e., the width of the stationary HF state), and ω is the angular frequency of the harmonic oscillator potential. One sees from (4.1) that the oscillation of the width is not harmonic at finite amplitudes, but becomes harmonic when the amplitude is infinitesimal.

When the Gauge Invariant Periodic condition is applied, we obtain a discrete set of solutions, corresponding to discrete values of the initial width D_0 . The energy spectrum of this discrete set of solutions is

$$E_n = 2 \hbar \omega \left(n + \frac{1}{2} \right). \quad (4.2)$$

The exact eigenenergies of the system is

$$E_n^{\text{exact}} = \sqrt{2} \hbar \omega \left(n + \frac{1}{2} \right), \quad (4.3)$$

where the factor $\sqrt{2}$ comes from the transformation from particle mass to reduced mass.

Comparing (4.2) with (4.3), we see that the Gauge Invariant Periodic spectrum has a spacing considerably larger than the spacing of the exact spectrum. The large spacing in (4.2) can be traced to the spurious center-of-mass motion in the TDHF solution. One can calculate the center-of-mass kinetic energy from the TDHF solutions. This energy will depend on time because of the nonlinearity of TDHF. But we can take the time average of

the center-of-mass energy and subtract it from E_n to obtain the average internal energy $\overline{E_n^{int}}$. We find that

$$\overline{E_n^{int}} = 1.5 \hbar \omega (n + \frac{1}{2}), \quad (4.4)$$

which can be compared with the exact spectrum (4.3), in which $\sqrt{2} = 1.414$ replaces the coefficient 1.5. Evidently (4.4) is a substantial improvement over (4.2).

V. CONCLUSION

This study implies that the Gauge Invariant Periodic TDHF solutions are a very promising approximate description of the exact Schroedinger eigenstates. They have the following promising features:

- (a) The wave functions have a structure very similar to the exact Schroedinger eigenstates.
- (b) They are orthogonal in the time average whenever they are non-degenerate.
- (c) They provide a discrete spectrum.
- (d) They require no assumption of small amplitudes or adiabaticity.

These features suggest them as an appropriate generalization of the small amplitude TDHF solutions to model the exact Schroedinger eigenstates.

Finally, we point out that in the discussion of the two-parameter model the assumption that Φ be a single determinant is never needed to obtain the Hamilton's equations. This implies that the concept of Gauge Invariant Periodicity has a much more general applicability than in the realm of TDHF. In fact it implies that it is applicable in all time-dependent approximate descriptions based upon the time-dependent variational principle.

APPENDIX

We seek solutions $p=p(\alpha,\beta)$ and $q=q(\alpha,\beta)$ from the pair of simultaneous equations (3.5), which is of the form

$$p \frac{\partial q}{\partial \alpha} = f(\alpha, \beta) \quad (\text{A.1a})$$

$$p \frac{\partial q}{\partial \beta} = g(\alpha, \beta). \quad (\text{A.1b})$$

Eqs. (A.1) are solved if we can find dq as a total differential such that

$$dq = \frac{f(\alpha, \beta)}{p(\alpha, \beta)} d\alpha + \frac{g(\alpha, \beta)}{p(\alpha, \beta)} d\beta. \quad (\text{A.2})$$

Eq. (A.2) is a Pfaffian differential equation, i.e.

$$f(\alpha, \beta)d\alpha + g(\alpha, \beta)d\beta - p(\alpha, \beta)dq = 0, \quad (\text{A.3})$$

whose integrability is determined by the necessary and sufficient condition [10],

$$X \cdot \nabla \times X = 0, \quad (\text{A.4})$$

where $X=(f,g,-p)$ and $\nabla=(\partial/\partial\alpha, \partial/\partial\beta, \partial/\partial q)$. But, condition (A.4) leads to the following first order linear equation for $p(\alpha,\beta)$:

$$g \frac{\partial p}{\partial \alpha} - f \frac{\partial p}{\partial \beta} + p \left(\frac{\partial f}{\partial \beta} - \frac{\partial g}{\partial \alpha} \right) = 0, \quad (\text{A.5})$$

which always possesses a solution [10].

Therefore, in order to solve (A.1), one can first solve (A.5) for $p(\alpha,\beta)$. Then substitute $p(\alpha,\beta)$ into the Pfaffian equation (A.3) which is now guaranteed to be integrable and whose solution gives $q(\alpha,\beta)$

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