Calculation of collective energies from periodic time-dependent Hartree-Fock solutions

Ismail Zahed*
Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Michel Baranger
Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
and Division de Physique Théorique, Institut de Physique Nucléaire, F-91406 Orsay, France
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A periodic time-dependent Hartree-Fock solution is used as the reference state for a diagrammatic expansion of the propagator. A discrete Fourier transform leads to a function of energy whose poles are the corresponding energy levels. Limiting the expansion to first-order diagrams leads to a new derivation of the Bohr-Sommerfeld—type quantization rule for collective states.

[NUCLEAR STRUCTURE Collective energies. Periodic time-dependent Hartree-Fock. Diagrammatic derivation of the Bohr-Sommerfeld quantization rule.]

I. MOTIVATION

Microscopic calculations of collective energy levels have often had as their starting point a static mean-field calculation of the ground state, using something like the Hartree-Fock or Brueckner-Hartree-Fock approximation. But one knows very well how to describe collective motion with a time-dependent mean field, as in the time-dependent Hartree-Fock (TDHF) approximation. The many successes of this approach are well known.[1,2] It does have some problems, however, one of which is that, from the collective point of view, it is a classical description with the consequences that, for bound states, need to be requantized, often in a rather arbitrary manner, and for scattering it is not rich enough to describe all the experimentally measured quantities.

This situation can be remedied if TDHF can be considered as the first step in a fully quantal theory, and this is just one of the results of the preceding paper.[3] We have shown in the preceding paper that it is possible, without changing things very much, to extend Feynman-Goldstone perturbation theory to the case where the basis is made up of time-dependent single-particle wave functions, all being solutions of the same time-dependent Schrödinger equation, which in the present case will be the TDHF equation. The result is a potentially exact formulation, provided the perturbation series converges, which of course is not a trivial matter. It is likely to be a much more accurate description of collective motion than the formulation starting from static Hartree-Fock, and to include it as a special case. In particular, approximations such as the random-phase approximation (RPA), which are based on static Hartree-Fock, cannot describe large amplitude collective motion, while the present approach can. Also, there is no adiabatic approximation in the present approach.

This paper is devoted to the derivation of the quantization rule for periodic TDHF solutions. The existence (or *possible* existence?) of these solutions has excited intense interest recently[4] because of their effective one-dimensional character and because of the analogy with classical mechanics. We use the Feynman-Goldstone expansion, in lowest order, to derive an unequivocal quantization rule for these solutions if they exist (and they do exist for simple models). This rule turns out to be identical to that previously derived by functional integrals,[5,6] and it is instructive and satisfying to see it derived in this completely new way. Later papers will develop corrections to this lowest order result.

II. PERIODIC TDHF SOLUTIONS

In a periodic TDHF solution,[2,7] the one-body density $\rho(t)$ is a periodic function of time with period τ

$$\rho(t+\tau)=\rho(t) \tag{1}$$

and frequency

$$\omega=2\pi/\tau\ . \tag{2}$$

Therefore, the single-particle potential $U(t)$ has period τ also. The single-particle states are solutions of the time-dependent Schrödinger equation in this potential. They are not periodic, but quasiperiodic, as in Bloch's or Floquet's theorem. This means

$$|\alpha(t+\tau)\rangle=e^{-i\theta_\alpha}|\alpha(t)\rangle\ , \tag{3}$$

where θ_α is a phase angle characteristic of the particular single-particle state. Obviously, these phases disappear in the construction of the one-body density as a sum over occupied states

$$\rho(t)=\sum_A |A(t)\rangle\langle A(t)| \ , \tag{4}$$

and $\rho(t)$ is truly periodic.

It is possible to define a variable λ_α having dimensions of energy by

$$\theta_\alpha=\lambda_\alpha\tau \ \text{(note : } \hbar=1) \ , \tag{5}$$

and to define $|\alpha^P(t)\rangle$, the periodic part of $|\alpha(t)\rangle$, by

$$|\alpha(t)\rangle=e^{-i\lambda_\alpha t}|\alpha^P(t)\rangle \ . \tag{6}$$

One checks immediately that $|\alpha^P(t)\rangle$ is truly periodic. We shall call λ_α the quasienergy of single-particle state α. It is similar to the "crystal momentum" of Bloch's theorem and it is defined up to a multiple of ω only. The time-dependent Schrödinger equation, written for $|\alpha^P(t)\rangle$, becomes

$$\left[i\frac{\partial}{\partial t}-K-U(t)\right]|\alpha^P(t)\rangle=-\lambda_\alpha|\alpha^P(t)\rangle \ . \tag{7}$$

One way of looking for periodic TDHF solutions[2,7] consists in solving the set of Eqs. (7) as one would the static HF equations, but with the added dimension of time and the added boundary condition that $|\alpha^P(t)\rangle$ has period τ. In this process, the value of τ is arbitrary and, although one may not find solutions for all possible τ, it becomes natural to expect that solutions will exist over a continuous range of τ, which is one of their characteristic features, and which reinforces the analogy with one-dimensional classical solutions.

Considering now the reference state $|\phi_0(t)\rangle$, which is the Slater determinant built out of the occupied single-particle states $|A(t)\rangle$, we find that it is quasiperiodic also,

$$|\phi_0(t+\tau)\rangle=e^{-i\Theta_0}|\phi_0(t)\rangle \ , \tag{8}$$

with

$$\Theta_0=\sum_A \theta_A \ . \tag{9}$$

The periodic part and the quasienergy of $|\phi_0(t)\rangle$ are defined by

$$|\phi_0(t)\rangle=e^{-i\Lambda_0 t}|\phi_0^P(t)\rangle \ , \tag{10}$$

with

$$\Lambda_0=\sum_A \lambda_A=\Theta_0/\tau \ . \tag{11}$$

We derive in the Appendix some variational properties of periodic TDHF solutions which will be useful in Secs. V and VI.

III. THE CHOICE OF BASIS

One of these periodic TDHF solutions will be our basis. Which one? One problem is that, if there are many degrees of freedom, hence several types of collective motion, we should be able to pick the TDHF periodic solution which describes the kind of collective motion we want to consider. In complicated cases, this could be very difficult. If we solve the problem as a four-dimensional HF problem, by iterating Eq. (7), how are we going to make the result converge toward the kind of collective motion we wish? In simple cases, on the other hand (for instance, the Lipkin model), it is very easy to see what to do.

Another question is associated with the continuous range of values of the period τ, as mentioned in Sec. II. Which of these should we use? This question has an approximate answer, which is interesting and important. From now on we shall assume that we are dealing with a one-parameter continuous family of periodic TDHF solutions. The parameter can be τ, or $\omega=2\pi/\tau$, or W, the energy, i.e., the expectation value of the exact Hamiltonian H for the TDHF wave function, which is well known to be time independent. All three of these parameters are related and equivalent. A possible relation between ω and W is shown in Fig. 1. When W is the energy of the HF ground state, ω is the RPA frequency. As W increases, ω changes. Viewed as a function of the collective coordinate, the TDHF wave function is a wave packet, i.e., a classical object, which is an approximate superposition of exact stationary states whose energies lie in the vicinity of W. Its frequency ω is an approximation to the level spacing, again for levels in the vicinity of W. Thus the curve $\omega(W)$ is an approximate description of the variation of the spacing of the collective levels with their excitation energy. It is clear, then, that W should be chosen to agree roughly with the energy of the level one is interested in. One will use a different W, i.e., a different basis with a different period, for calculations concerning each collective level. And since one does not know, at the start, the exact energy levels, one will need a quantization rule to fix, at least provisionally, the best value of W to be used for each level. This is the quantization rule which we shall derive in Sec. VI.

Note that, in principle, the Feynman-Goldstone expansion of Ref. 3 is exact irrespective of what we pick for W.

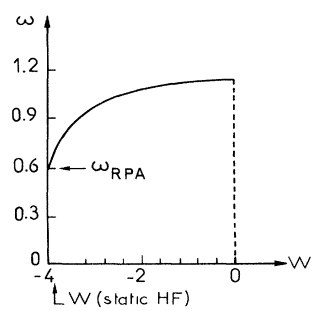

FIG. 1. The relation between ω and W for a Lipkin model (Ref. 10) ($N=8$, $\epsilon=1$, and $\chi=0.8$). In real nuclei, it is more usual for ω to decrease as W increases.

Its convergence, however, is obviously very much affected by W. Thus, the game is to pick as good a W as is possible at the outset, and this we shall do separately for each level, using the quantization rule. It can then be hoped that higher-order corrections will converge rapidly after this.

IV. THE CALCULATION OF BOUND STATE ENERGIES

Though the states of the basis are not stationary, the fact that they are quasiperiodic allows us to make a Fourier transformation to an energy variable. This transformation, however, is different from what is done in the usual case of a stationary basis.

In the usual case, the reference state ϕ_0 is stationary with unperturbed energy W_0, i.e.,

$$\langle \phi_0(T) | = \langle \phi_0(0) | e^{iW_0 T} . \tag{12}$$

One way to look for bound state energies is to calculate somehow the "reference-to-reference" matrix element of the propagator

$$\langle \phi_0(T) | e^{-iHT} | \phi_0(T) \rangle , \tag{13}$$

which by (12) can also be written

$$\langle \phi_0(0) | e^{-i(H-W_0)T} | \phi_0(0) \rangle . \tag{14}$$

Introducing as intermediate states the complete set of exact stationary states ψ_n with exact energies E_n, we can write (14) as

$$\sum_n | \langle \phi_0(0) | \psi_n \rangle |^2 e^{-i(E_n - W_0)T} . \tag{15}$$

Then we Fourier integrate over positive times with an energy variable E, and we get the formula

$$-i \int_0^\infty dT\, e^{i(E-W_0)T} \langle \phi_0(T) | e^{-iHT} | \phi_0(0) \rangle = \sum_n \frac{| \langle \phi_0(0) | \psi_n \rangle |^2}{E - E_n} . \tag{16}$$

The idea is to find some diagrammatic approximation for the matrix element on the left-hand side as a function of T, Fourier transform it, look for the poles in E, which should be approximations to the true energy levels E_n, while the residues should be approximations to $| \langle \phi_0(0) | \psi_n \rangle |^2$.

In the present case, $\langle \phi_0(T) |$ is not an harmonic function of T such as (12). But if T is a multiple of the period τ, then things are simple again and we have

$$\langle \phi_0(N\tau) | = \langle \phi_0(0) | e^{i\Lambda_0 N\tau} , \tag{17}$$

and therefore

$$\langle \phi_0(N\tau) | e^{-iHN\tau} | \phi_0(0) \rangle = \sum_n | \langle \phi_0(0) | \psi_n \rangle |^2 e^{-i(E_n - \Lambda_0)N\tau} . \tag{18}$$

This time we do a discrete Fourier transform, using the formula

$$\sum_{N=0}^{\infty} e^{iNx} = (1 - e^{ix})^{-1} , \tag{19}$$

and we write, instead of (16),

$$-i\tau \sum_{N=0}^{\infty} e^{i(E-\Lambda_0)N\tau} \langle \phi_0(N\tau) | e^{-iHN\tau} | \phi_0(0) \rangle = \sum_n \frac{-i\tau | \langle \phi_0(0) | \psi_n \rangle |^2}{1 - \exp i(E - E_n)\tau} . \tag{20}$$

The right-hand side has poles at

$$E = E_n + m\omega , \tag{21}$$

where m is any integer, positive, negative, or zero. These additional ghost poles are the price one has to pay for using the discrete instead of the continuous Fourier transform. The residue for each pole is just $| \langle \phi_0(0) | \psi_n \rangle |^2$, the same as earlier.

Our strategy is then as follows. We do an approximate diagrammatic calculation of $\langle \phi_0(N\tau) | e^{-iHN\tau} | \phi_0(0) \rangle$ for all positive integer N, we perform the Fourier sum in the left-hand side of (20), we look for its poles and residues in E, and we compare it with the right-hand side of (20) which contains the exact poles and residues. We shall now apply this strategy to a first-order calculation of the propagator matrix element.

V. FIRST-ORDER CALCULATION

The propagator matrix element is a sum of products of disconnected clusters, as shown in Fig. 2. The exponentiation theorem[8] states that this equals the exponential of the sum of all distinct single clusters, as shown also in Fig. 3. There are two first-order clusters only, which are shown in Fig. 3. Their numerical value, including the symmetry factor of $\frac{1}{2}$ for the "double bubble," is

$$-i \int_0^{N\tau} dt \left[\tfrac{1}{2} \sum_{AB} \langle A(t)B(t) | \tilde{V} | A(t)B(t) \rangle - \sum_A \langle A(t) | U(t) | A(t) \rangle \right] . \tag{22}$$

Because of the diagonal nature of the matrix elements, the integrand is periodic of period τ. Also, according to the usual Hartree-Fock definition[3] of $U(t)$, the first term can-

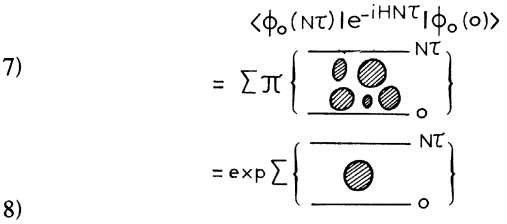

FIG. 2. Diagrammatic expansion of the reference-to-reference propagator matrix element and exponentiation theorem.

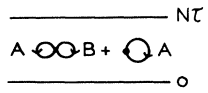

FIG. 3. The two first-order diagrams. The one-body vertex stands for $-U(t)$.

cels half of the second term. Hence these diagrams are equal to

$$iN\int_0^\tau dt\tfrac{1}{2}\sum_A \langle A(t)\,|\,U(t)\,|\,A(t)\rangle\ . \tag{23}$$

One finds easily, using the TDHF equations, that this is the same as

$$iNS = iN(J - W\tau)\ , \tag{24}$$

where S and J are the two actions defined in Eqs. (A15) and (A27) of the Appendix, respectively. Thus, this approximation to the propagator matrix element is

$$e^{iN(J-W\tau)}\ . \tag{25}$$

The Fourier sum on the left-hand side of Eq. (20) is then easily performed and yields

$$-i\tau[1-\exp i(E\tau-\Lambda_0\tau+J-W\tau)]^{-1} = -i\tau[1-\exp i(E\tau+J^P-W\tau)]^{-1}\ , \tag{26}$$

where J^P is the quantity defined in Eq. (A28). This has poles for values of E given by

$$E = W - J^P/\tau + m\omega\ , \tag{27}$$

and all the residues are unity. When we try to compare these poles with the exact ones, Eq. (21), we are faced with a problem.

VI. THE QUANTIZATION RULE

The problem is this. The exact poles (21) depend on two discrete parameters, n and m. The approximate poles (27) depend on one discrete parameter only, m. How should the identification be made? The answer lies in looking at the residues.

But before this, note that both sets of poles also depend on one continuous parameter W (or ω, or τ) which, so far, we do not know how to determine. This dependence is relatively trivial for the exact poles, but it is essential for the approximate ones.

We begin by plotting the approximate poles (27), using ω as the continuous variable, i.e., we plot

$$E = W(\omega) - \omega J^P(\omega)/2\pi + m\omega\ . \tag{28}$$

This is shown in Fig. 4(a) for a particular example. Each curve corresponds to a particular value of m. Since all residues are unity, the entire curves are presumed to be meaningful.

In Fig. 4(b), we plot the exact poles (21), a double family of straight lines of slope m. These lines are not equally meaningful everywhere, because the residue $|\langle\phi_0(0)\,|\,\psi_n\rangle|^2$ might sometimes be very small. According to the argument we gave in Sec. III, which looks upon TDHF as a classical approximation to the collective motion, we expect the overlap $\langle\phi_0(0)\,|\,\psi_n\rangle$ to be large when W is in the vicinity of E_n and small otherwise. Thus, for the lowest possible W, the overlap with ψ_0 is largest. As W increases, the overlap with ψ_1 becomes the largest one, and as W increases some more, the overlap with ψ_2 becomes largest, etc., ... Hence, we must single out, among the many dashed lines of Fig. 4(b), those lines which are issued from level E_0 if W is small, the lines issued from level E_1 when W is larger, and the lines issued from level E_2 when W is still larger, etc., ... These pieces of lines are shown as solid segments on the figure and, when considered together, they form curved lines which begin to resemble very strongly the curves of Fig. 4(a). The situation becomes even clearer when we switch to the variable ω against which the curves are plotted. According to the argument of Sec. III, the levels E_n with large residues are the ones for which the level spacing corresponds to the value of ω. If we now look for the intersection of the line $E(n,m)$ with the line $E(n+1,m-1)$, we get the condition

$$E_n + m\omega = E_{n+1} + (m-1)\omega \tag{29}$$

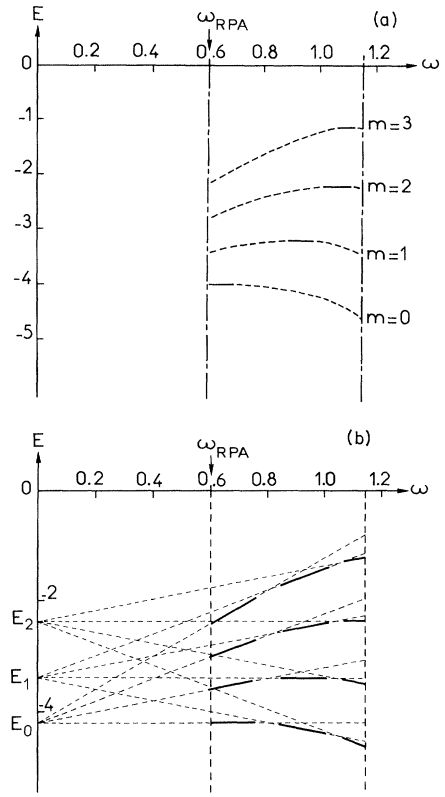

FIG. 4. The bound state poles E vs ω, for the same Lipkin model as Fig. 1, (a) shows $E(m,\omega)$ according to Eq. (28). (b) shows as dashed straight lines the double family $E(n,m,\omega)$ according to Eq. (21). The dashed lines have been replaced by solid segments in those regions of ω where the residue is expected to be large. E_0, E_1, and E_2 are the exact energy levels.

or

$$E_{n+1}-E_n=\omega\ , \tag{30}$$

which is precisely the condition on the level spacing. Going to the limit of large quantum numbers, we see that the curves we want, for purposes of comparison with Fig. 4(a), are the envelopes of the families of straight lines $E(n+p,m-p)$ for variable p. These envelopes do indeed look very similar to the curves of Fig. 4(a), the small remaining discrepancy owing to the neglect of higher-order diagrams in Fig. 4(a).

Once this identification of the two sets of curves has been made, the determination of the approximate energy levels is easy since, according to Fig. 4(b), they correspond to those values of E for which the curve $E(\omega)$ has a horizontal slope. Hence, we must set the derivative of (28) equal to zero

$$\frac{dE}{d\omega}=\frac{dW}{d\omega}-\frac{J^P(\omega)}{2\pi}-\frac{\omega}{2\pi}\frac{dJ^P}{dW}\frac{dW}{d\omega}+m=0\ . \tag{31}$$

According to Eq. (A31), $dJ^P/dW=\tau$, while $\omega/2\pi=\tau^{-1}$, hence we are left with

$$J^P=2\pi m\ . \tag{32}$$

Equation (28) shows then that $E=W$. Thus, we reach the result: the approximate energy levels are those values of W which satisfy

$$J^P(W)=2\pi m\ , \tag{33}$$

where m is an integer. This is the Bohr-Sommerfeld—type quantization rule,[6] derived in a completely new way.

Higher-order corrections to this have been worked out and we shall publish them in a forthcoming paper. We shall also present a detailed application to the Lipkin model.

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APPENDIX: PERIODIC TDHF AS A VARIATIONAL PROBLEM

We begin by reviewing some well-known variational properties of a classical system with coordinates q_n, momentum conjugates p_n, and Hamiltonian $H(p_n,q_n)$. Hamilton's action is

$$S=\int_{t_0}^{t_1}dt\left\{\sum_n p_n(t)\dot{q}_n(t)-H[p_n(t),q_n(t)]\right\}\ . \tag{A1}$$

If one calculates δS for arbitrary variations $\delta p_n(t),\delta q_n(t)$ satisfying

$$\delta q_n(t_0)=\delta q_n(t_1)=0\ , \tag{A2}$$

one finds after one integration by parts

$$\delta S=\int_{t_0}^{t_1}dt\sum_n\left[\delta p_n\left[\dot{q}_n-\frac{\partial H}{\partial p_n}\right]-\delta q_n\left[\dot{p}_n+\frac{\partial H}{\partial q_n}\right]\right]\ . \tag{A3}$$

Setting $\delta S=0$ yields Hamilton's equations of motion; this is Hamilton's principle. Note that S can also be written

$$S=\int\left[\sum_n p_n dq_n-H(p_n,q_n)dt\right]\ , \tag{A4}$$

where the integral is taken along the trajectory in phase space.

Now we consider only periodic trajectories of variable period τ, and we take one period as the integration interval for S. We replace the time t by a cyclic parameter η varying from 0 to 1, i.e., we write $t=\eta\tau$. Then, p_n and q_n are periodic functions of η of period 1 (at least, this is so if q_n are Cartesian coordinates). The action is then

$$S=\int_0^1 d\eta\left\{\sum_n p_n\frac{dq_n}{d\eta}-H[p_n(\eta),q_n(\eta)]\tau\right\}\ . \tag{A5}$$

If one calculates δS for arbitrary variations $\delta p_n(\eta),\delta q_n(\eta)$ which keep the functions periodic, and if one also varies τ, one finds after one integration by parts

$$\delta S=\int_0^1 d\eta\sum_n\left[\delta p_n\left[\frac{dq_n}{d\eta}-\tau\frac{\partial H}{\partial p_n}\right]-\delta q_n\left[\frac{dp_n}{d\eta}+\tau\frac{\partial H}{\partial q_n}\right]\right]-\delta\tau\int_0^1 d\eta H(\eta)\ . \tag{A6}$$

When this is evaluated for correct trajectories, the coefficients of δp_n and δq_n vanish by virtue of Hamilton's equations, and again by virtue of these equations $H(\eta)$ is a constant, the energy W; therefore one gets

$$\delta S=-W\delta\tau \text{ or } \partial S/\partial\tau=-W\ . \tag{A7}$$

This tells us how the action S varies when we go from a correct trajectory to another correct trajectory with a different period. Let us introduce the reduced action J (sometimes called Maupertuis's action), which is the first part of S,

$$J=\int_0^1 d\eta\sum_n p_n\frac{dq_n}{d\eta}=\oint\sum_n p_n dq_n\ . \tag{A8}$$

We see that, for correct trajectories,

$$J=S+W\tau\ , \tag{A9}$$

therefore

$$\delta J=\delta S+W\delta\tau+\tau\delta W\ , \tag{A10}$$

therefore, by virtue of (A7),

$$\delta J=\tau\delta W \text{ or } \partial J/\partial W=\tau\ . \tag{A11}$$

This tells us how the action J varies when we go from a correct trajectory to another correct trajectory with a different energy.

We can now proceed to TDHF. Kerman and Koonin[9] have pointed out that it can be formulated in a way almost identical to the above Hamiltonian formulation of classical mechanics. The action is

$$S=\int_{t_0}^{t_1}dt\left\{\sum_A i\langle\varphi_A(t)\,|\,\dot{\varphi}_A(t)\rangle-H[\langle\varphi_A(t)\,|\,,|\,\varphi_A(t)\rangle]\right\}, \tag{A12}$$

which is a real quantity. The role of p_n and q_n is played by the bras and kets of the occupied single-particle states φ_A, which have to be varied independently, and $H[\langle\varphi_A(t)\,|\,,|\,\varphi_A(t)\rangle]$ is the expectation value of the exact Hamiltonian for the Slater determinant. For arbitrary variations of $\langle\varphi_A\,|$ and $|\,\varphi_A\rangle$ satisfying the normalization condition and

$$|\,\delta\varphi_A(t_0)\rangle=|\,\delta\varphi_A(t_1)\rangle=0\ , \tag{A13}$$

one finds after one integration by parts

$$\delta S=\int_{t_0}^{t_1}dt\sum_A[\langle\delta\varphi_A\,|\,i\dot{\varphi}_A-(K+U)\varphi_A\rangle-\langle i\dot{\varphi}_A+\varphi_A(K+U)\,|\,\delta\varphi_A\rangle]\ . \tag{A14}$$

Setting $\delta S=0$ yields the TDHF equations of motion.

Now we consider only periodic trajectories of variable period τ, and we do the time integral over one period. Once again we set $t=\eta\tau$, so that we write

$$S=\int_0^1 d\eta\left\{\sum_A i\left\langle\varphi_A(\eta)\left|\frac{d\varphi_A}{d\eta}\right.\right\rangle-H[\langle\varphi_A(\eta)|\ ,|\,\varphi_A(\eta)\rangle]\tau\right\}. \tag{A15}$$

We calculate δS for arbitrary variations of $\langle\varphi_A\,|$ and $|\,\varphi_A\rangle$ which keep the one-body density periodic, and we also vary τ. Things are a little different from previous results, however, because the $|\,\varphi_A(\eta)\rangle$'s are not periodic any more, but quasiperiodic. Let us do the variation in detail

$$\delta S=\int_0^1 d\eta\sum_A\left[i\left\langle\delta\varphi_A\left|\frac{d\varphi_A}{d\eta}\right.\right\rangle+i\left\langle\varphi_A\left|\delta\frac{d\varphi_A}{d\eta}\right.\right\rangle-\tau\left\langle\delta\varphi_A\left|\frac{\partial H}{\partial\langle\varphi_A\,|}\right.\right\rangle-\tau\left\langle\frac{\partial H}{\partial\,|\,\varphi_A\rangle}\right|\delta\varphi_A\right\rangle\Bigg]-\delta\tau\int_0^1 d\eta\,H(\eta)\ . \tag{A16}$$

The integration by parts is the following:

$$\int_0^1 d\eta\left\langle\varphi_A\left|\delta\frac{d\varphi_A}{d\eta}\right.\right\rangle=\langle\varphi_A\,|\,\delta\varphi_A\rangle\,|_0^1-\int_0^1 d\eta\left\langle\frac{d\varphi_A}{d\eta}\right|\delta\varphi_A\right\rangle\ . \tag{A17}$$

The integrated part does not vanish. Rather, we have

$$|\,\varphi_A(1)\rangle=e^{-i\theta_A}\,|\,\varphi_A(0)\rangle\ , \tag{A18}$$

$$|\,\delta\varphi_A(1)\rangle=-i\delta\theta_A\,|\,\varphi_A(1)\rangle+e^{-i\theta_A}\,|\,\delta\varphi_A(0)\rangle\ , \tag{A19}$$

$$\langle\varphi_A(1)\,|\,\delta\varphi_A(1)\rangle=-i\delta\theta_A+\langle\varphi_A(0)\,|\,\delta\varphi_A(0)\rangle\ , \tag{A20}$$

$$\langle\varphi_A\,|\,\delta\varphi_A\rangle\,|_0^1=-i\delta\theta_A\ . \tag{A21}$$

Hence the variation of S is

$$\delta S=\int_0^1 d\eta\sum_A\left[\left\langle\delta\varphi_A\left|i\frac{d\varphi_A}{d\eta}-\tau(K+U)\varphi_A\right.\right\rangle-\left\langle i\frac{d\varphi_A}{d\eta}+\varphi_A(K+U)\tau\right|\delta\varphi_A\right\rangle\Bigg]+\sum_A\delta\theta_A-\delta\tau\int_0^1 d\eta\,H(\eta)\ . \tag{A22}$$

If we restrict ourselves to correct TDHF trajectories, the coefficients of $\langle\delta\varphi_A\,|$ and $|\,\delta\varphi_A\rangle$ vanish by virtue of the TDHF equations, and the energy $H(\eta)$ is a constant W; hence we can write, using Eq. (9),

$$\delta S=\delta\Theta_0-W\delta\tau\ . \tag{A23}$$

Let us now define an action S^P identical to S, but built upon the periodic part φ_A^P of the occupied single-particle states [see Eq. (6)], in other words

$$S^P=\int_0^1 d\eta\left\{\sum_A i\left\langle\varphi_A^P(\eta)\left|\frac{d\varphi_A^P}{d\eta}\right.\right\rangle-H[\langle\varphi_A^P(\eta)|\ ,|\,\varphi_A^P(\eta)\rangle]\tau\right\}. \tag{A24}$$

One sees easily

$$S^P=S-\Theta_0\ , \tag{A25}$$

and therefore, for correct TDHF trajectories,

$$\delta S^P = -W\delta\tau \text{ or } \partial S^P/\partial\tau = -W \,. \tag{A26}$$

This gives us the change in S^P when we go from one TDHF solution to another TDHF solution with a different period. Finally, we introduce both forms of Maupertuis's action

$$J = \int_0^1 d\eta \sum_A i\left\langle \varphi_A(\eta) \left| \frac{d\varphi_A}{d\eta} \right\rangle \right. , \tag{A27}$$

$$J^P = \int_0^1 d\eta \sum_A i\left\langle \varphi_A^P(\eta) \left| \frac{d\varphi_A^P}{d\eta} \right\rangle \right. = J - \Theta_0 \,. \tag{A28}$$

We have for correct TDHF trajectories

$$J^P = S^P + W\tau \,, \tag{A29}$$

$$\delta J^P = \delta S^P + W\delta\tau + \tau\delta W \,, \tag{A30}$$

therefore, by virtue of (A26),

$$\delta J^P = \tau\delta W \text{ or } \partial J^P/\partial W = \tau \,. \tag{A31}$$

This formula gives us the change in J^P when we go from one periodic TDHF solution to another one with a different energy. Sometimes it can also be used to calculate the period, in those cases where J^P can be evaluated from Eq. (A28) without reference to time.

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*Present address: The Niels Bohr Institute, DK-2100 Copenhagen Ø, Denmark.

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