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Time-dependent mean-field theory and quantized bound states

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A theory is presented in which approximations to quantum observables are obtained by applying the stationary-phase approximation to an exact functional integral representation of the many-body evolution operator. The requirement that the leading correction to the stationary-phase approximation vanish leads to a time-dependent Hartree-Fock mean field. Application of the theory to the Fourier transform of the trace of the evolution operator and the study of its poles yields quantized bound states with large amplitude. The theory is shown to reproduce the familiar static Hartree-Fock and random-phase approximations in the appropriate limits and yields an excellent approximation to the entire spectrum of the exactly solvable Lipkin model.

[NUCLEAR STRUCTURE Derivation of time-dependent mean-field theory from functional integral representation. Quantum theory of large amplitude collective motion. Application to Lipkin model.]

I. INTRODUCTION

The concept of a mean field plays an enigmatic role in the physics of nonrelativistic many-body sytems. Whereas the mean field is crucial to the nuclear shell model, and thus one's entire understanding of nuclear structure, and provides the foundation for understanding many solid state and condensed matter phenomena, it does not exist as a fundamental entity. It is purely an artificial theoretical construction; it cannot even be uniquely defined, let alone measured. Thus, it is inevitable that serious questions of principle arise in the application of a mean-field approximation; such as the time-dependent Hartree-Fock approximation (TDHF) to quantum processes.

This present work therefore addresses the problem of developing approximations to quantum observables in a formalism which retains the physical insight provided by a mean field. Rather than asking how to interpret the time-dependent mean-field solution to a specific initial value problem, we begin with an exact quantum expression for an observable and develop a mean-field approximation to it. The resulting theory is thus free of ambiguities of interpretation and philosophy, and subject only to well-posed questions concerning the accuracy of approximation. Given the conviction that semiclassical pictures of collective vibration, rotations, and heavy ion collisions embody much of the correct physics, we believe it is extremely valuable to be able to embed this understanding in a proper quantum framework.

Motivated by advances in applying functional integral techniques to quantum field theory, the mean field is introduced through a functional integral representation of the exact evolution operator following the approach of Ref. 1. Evaluation of the functional integral in the stationary-phase approximation then yields a mean-field approximation to any observable expressed in terms of the evolution operator. The range of applicability of this method is thus in principle extremely broad, encompassing bound state energies and expectation values of few-body operators, the density of continuum states, tunneling decay of unstable states, and scattering processes.

This present work is devoted to the problem of obtaining the Hartree-Fock (HF) mean field, rather than the Hartree field, from the stationary-phase approximation (SPA) and to calculation of the bound state spectrum by evaluation of the Fourier transform of the trace of the evolution operator. The exchange term in the mean-field approximation is obtained by exploiting the freedom to write alternative exact functional integral expressions which yield different results in the lowest order SPA. The particular choice which yields the physically appealing HF mean field also has the advantage that the leading correction to the SPA vanishes. The calculation of the bound state spectrum follows closely the pioneering work of Dashen, Hausslacher, and Neveu.[2] In addition to recovering familiar HF and random-phase approximation (RPA) limits, we derive a quantized theory of large amplitude collective motion. Other applications will be published subsequently.

Corrections to the stationary-phase approximation can only be implemented in very low order, if at all, giving rise to several significant open questions. In all but the most artificial model problems, there is no small expansion parameter

(other than $\hbar$) so the quantitative validity is difficult to assess. Although the theory is formulated in terms of matrix elements of the evolution operator, as in any many-body theory, we may at most hope to calculate reliable expectation values of few-body operators. To the present order of approximation, the theory is particularly deficient in dealing with the short-range correlations required by the repulsive core of the nucleon-nucleon interaction or the potentials between atoms in liquid helium. For present purposes, we simply assume that the bare potential may ultimately be replaced by an effective interaction or pseudopotential such as the Skyrme interaction, and relegate the rigorous formulation in terms of effective operators to subsequent research. Finally, we note that arbitrary choices will often arise when alternative exact expressions yield differing lowest order approximations. Whereas one can manipulate the formalism to produce specific intuitively appealing results or to minimize a particular higher order correction, there is no criterion at present for generating an optimal approximation.

In many respects, this work is a complementary alternative to the coupled-cluster hierarchy, which also addresses systematic corrections to the mean-field approximation.[3] The coupled-cluster theory focuses directly on the two-body correlations which are beyond the scope of the present work. The functional integral approach, on the other hand, emphasizes the problem of quantization of collective motion far more directly than the coupled-cluster method. The present theory is thus especially relevant for bound states and relatively low energy nuclear dynamics. At higher energies, where two-body collisions and particle emission from hard core interactions are crucial, the coupled-cluster description becomes natural. Whereas establishing detailed correspondence with perturbation theory is in either case difficult for dynamic problems, it is more straightforward with the coupled-cluster language. The fact that the functional integral formulation is essentially nonperturbative, however, is an asset in formulating tunneling problems such as spontaneous fission.

The organization of this paper is as follows. Section II addresses the question of how best to define the mean field and explores certain simple corrections to the stationary-phase approximation. A general technique for approximating eigenstates is presented in Sec. III, resulting in self-consistent periodic TDHF equations subject to a quantization condition.[17] Linearization of this theory is shown to reproduce the familiar random-phase approximation (RPA). In Sec. IV the general equations are solved for the Lipkin model and conclusions and prospects for subsequent applications are discussed in Sec. V.

II. ALTERNATIVE MEAN-FIELD APPROXIMATIONS

A. The simplest mean-field approximation

One simple way of rewriting the second quantized Hamiltonian

$$H=\frac{1}{2m}\int \nabla\psi^\dagger(x)\nabla\psi(x)dx + \tfrac{1}{2}\int\int dx\,dx'\psi^\dagger(x)\psi^\dagger(x') \times V(x-x')\psi(x')\psi(x) \tag{2.1}$$

is

$$H=K+\tfrac{1}{2}\int\int dx\,dx'\hat{\rho}(x)V(x-x')\hat{\rho}(x'), \tag{2.2}$$

where $\hat{\rho}(x)$ is the density operator $\psi^\dagger(x)\psi(x)$. We use units with $\hbar=1$, and K includes the self-interaction term

$$K\equiv\frac{1}{2m}\int \nabla\psi^\dagger(x)\nabla\psi(x)dx-\tfrac{1}{2}V(0)\int dx\hat{\rho}(x). \tag{2.3}$$

The interaction representation evolution operator is then given by the time-ordered product

$$U(t_f,t_i)=\tau\exp\left[-\frac{i}{2}\int_{t_i}^{t_f}dt\int\int dx\,dx'\hat{\rho}(x,t) \times V(x-x')\hat{\rho}(x',t)\right], \tag{2.4}$$

where τ will always denote the time-ordering operator and

$$\hat{\rho}(x,t)\equiv e^{iKt}\hat{\rho}(x)e^{-iKt}. \tag{2.5}$$

As shown in Ref. 1, use of the Hubbard-Stratonovich transformation[4] allows one to replace the exact evolution operator containing two-body operators by a functional integral over expressions involving one-body operators:

$$\langle f|U(t_f,t_i)|i\rangle=\int D[\sigma]\exp\left(\frac{i}{2}\int\int\int\int\sigma V\sigma\right) \times\langle f|U_\sigma(t_f,t_i)|i\rangle, \tag{2.6}$$

where

$$U_\sigma(t_f,t_i)=\tau\exp\left(-i\int\int\int\sigma V\hat{\rho}\right), \tag{2.7}$$

and in cases where no confusion should arise, we define

$$\int\int\int fVg \equiv \int_{t_i}^{t_f} dt \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' f(x,t) V(x-x') g(x',t), \tag{2.8}$$

$$|i\rangle \equiv |\Phi_i(t_i)\rangle, \tag{2.9}$$

and

$$\langle f| \equiv \langle \Phi_f(t_f)| . \tag{2.10}$$

For the derivation of (2.6) it was appropriate to use the interaction representation. When convenient, subsequently, we shall also use the Schrödinger representation without specific comment. The measure $D[\sigma]$ in (2.6) is as defined in Ref. 1. Equation (2.6) may be rewritten in terms of the effective action

$$S_{\text{eff}}[\sigma] \equiv \tfrac{1}{2}\int\int\int \sigma V \sigma - i \ln\left\langle f\left|\tau \exp\left(-i\int\int\int \sigma V\hat{\rho}\right)\right|i\right\rangle, \tag{2.11}$$

where the lowest order stationary-phase approximation yields

$$\langle f|U|i\rangle = \int D[\sigma] e^{iS_{\text{eff}}[\sigma]} \approx e^{iS_{\text{eff}}[\sigma^0]}. \tag{2.12}$$

In (2.12) σ^0 is found by solving the equation[1]

$$\sigma^0(x,t) = \frac{\langle f|\tau\hat{\rho}(x,t)\exp(-i\int\int\int\sigma^0 V\hat{\rho})|i\rangle}{\langle f|\exp(-i\int\int\int\sigma^0 V\rho)|i\rangle} = \frac{\langle \Phi_f(t)|\hat{\rho}(x,t)|\Phi_i(t)\rangle}{\langle\Phi_f(t)|\Phi_i(t)\rangle}, \tag{2.13}$$

where the time-dependent wave functions are defined as

$$|\Phi_i(t)\rangle = U_{\sigma 0}(t,t_i)|i\rangle, \quad \langle\Phi_f(t)| = \langle f|U_{\sigma 0}(t_f,t). \tag{2.14}$$

Equation (2.12) gives a mean-field approximation for the matrix elements of the many-body evolution operator U. Unfortunately, in the present simple form this approximation does not take proper account of the particle statistics in the many-body system. This fact becomes more transparent if one considers the situation where $|i\rangle$ and $|f\rangle$ are determinants and

$$|\Phi_f(t)\rangle = |\Phi_i(t)\rangle = |\Phi(t)\rangle .$$

Since $U_{\sigma 0}$ is an evolution operator in a one-body potential it is obvious that $|\Phi(t)\rangle$ in this case is also a determinant:

$$|\Phi(t)\rangle \equiv \frac{1}{\sqrt{A!}}\sum_P (-1)^P \prod_{j=1}^{A} \phi_P(x_j,t), \tag{2.15}$$

where the single-particle wave functions are orthonormal and satisfy the time-dependent equation

$$i\dot{\phi}_j(x,t) = \left[\frac{p^2}{2m} - \tfrac{1}{2}V(0) + \int V(x-x')\sigma^0(x',t)dx'\right]\phi_j(x,t). \tag{2.16}$$

The expression for σ^0 is now simply

$$\sigma^0(x,t) = \langle\Phi(t)|\hat{\rho}(x,t)|\Phi(t)\rangle = \sum_{j=1}^{A} |\phi_j(x,t)|^2 . \tag{2.17}$$

Thus, the single-particle wave functions evolve in the Hartree potential

$$V_{\text{Hartree}}(x) = \int \sigma^0(x',t)V(x-x')dx' . \tag{2.18}$$

In this special simple case, we see quite directly that although we used antisymmetrized wave functions, nevertheless we obtained the Hartree rather than the Hartree-Fock mean field. In fact, whether we antisymmetrize, symmetrize, or simply write a product wave function, the character of the mean field is unaffected.

The fact that the mean field depends on statistics in the Hartree sense only constitutes a serious conceptual as well as practical problem. Certainly, in the case of nuclear forces, for which exchange matrix elements are systematically larger than direct matrix elements, such a limitation would be catastrophic. Conceptually, it is quite disturbing not to understand the absence of exchange. Is the present approach intrinsically limited to bosons with a more complicated formulation being required for fermions? Or, is there additional, unutilized freedom with which one can impose a more desirable mean field? In order to clarify these issues and obtain insight into generating alternative mean-field theories, it is useful to explicitly calculate the quadratic corrections to the stationary-phase approximation.

B. Quadratic corrections to the stationary-phase approximation

We consider corrections to the zeroth order stationary-phase result, Eq. (2.12), by expanding $S_{\text{eff}}[\sigma]$ through second order in variations of σ from the stationary solution σ^0. Defining $\zeta \equiv \sigma - \sigma^0$ and using the fact that the linear term vanishes by the stationarity condition (2.13), we have

$$\int D[\sigma]e^{iS_{\text{eff}}[\sigma]} \simeq \int D[\xi]\exp\left[iS_{\text{eff}}[\sigma^0] + \frac{i}{2}\int dx\,dx'\,dt\,dt' \frac{\delta^2 S_{\text{eff}}}{\delta\sigma(x,t)\delta\sigma(x't')}\xi(x,t)\xi(x't')\right]$$

$$= \left[\frac{\det[V(x-x')\delta(t-t')]}{\det\left[\dfrac{\delta^2 S_{\text{eff}}}{\delta\sigma(x,t)\delta\sigma(x't')}\right]}\right]^{1/2} e^{iS_{\text{eff}}[\sigma^0]}, \tag{2.19}$$

where the last identity is derived in Appendix A. The determinants in (2.19) are understood in the functional sense with respect to the matrix "indices" x, t and x', t', the spin-isospin indices are suppressed throughout the subsection. The second functional derivative of S_{eff}, Eq. (2.11), is evaluated at the stationary value of $\sigma = \sigma^0$, with the result

$$\frac{\delta^2 S_{\text{eff}}}{\delta\sigma(x,t)\delta\sigma(x't')} = \delta(t-t')V(x-x') - \int\int ds\,ds' V(x-s)V(x'-s')D_0(st;s't'), \tag{2.20}$$

where D_0 is defined by

$$iD_0(st;s't') \equiv \frac{\langle f|\tau\hat{\rho}(st)\hat{\rho}(s't')\exp -i\int\sigma^0 V\hat{\rho}|i\rangle}{\langle f|\tau\exp -i\int\sigma^0 V\rho|i\rangle} - \frac{\langle f|\tau\hat{\rho}(st)\exp -i\int\sigma^0 V\hat{\rho}|i\rangle\langle f|\tau\hat{\rho}(s't')\exp -i\int\sigma^0 V\hat{\rho}|f\rangle}{\langle f|\tau\exp -i\int\sigma^0 V\rho|i\rangle\langle f|\tau\exp -i\int\sigma^0 V\rho|i\rangle}. \tag{2.21}$$

The quantity D_0 is a natural generalization of the familiar density correlation function.[5] Rewriting the second functional derivative in an obvious matrix notation

$$\frac{\delta^2 S_{\text{eff}}}{\delta\sigma(x,t)\delta\sigma(x't')} = \int\int dx''dt''\delta(t-t'')V(x-x'')[\delta(t''-t')\delta(x''-x')$$
$$+ \int\int dx'''dt'''D_0(x''t'';x'''t''')V(x'''-x')\delta(t'''-t')] \equiv [V\delta][1 - D_0(V\delta)] \tag{2.22}$$

and using the matrix identity $\det A = \exp(\operatorname{tr}\ln A)$, we obtain the quadratic correction factor

$$\left[\frac{\det(V\delta)}{\det\dfrac{\delta^2 S_{\text{eff}}}{\delta\sigma\delta\sigma}}\right]^{1/2} = \{\det[1 - D_0(V\delta)]\}^{-1/2} = \exp\{-\tfrac{1}{2}\operatorname{tr}\ln[1 - D_0(V\delta)]\} = \exp\tfrac{1}{2}\sum_{n=1}^{\infty}\operatorname{tr}\frac{1}{n}[D_0(V\delta)]^n. \tag{2.23}$$

The result (2.23) is easily interpreted in the case of static stationary solutions of the theory, for which the mean-field σ^0 is independent of time

$$\sigma^0(x) = \sum_{j=1}^{A}\psi_j^*(x)\psi_j(x) \tag{2.24}$$

and the single-particle wave functions satisfy

$$\left[\frac{p^2}{2m} - \tfrac{1}{2}V(0) + \int V(x-x')\sigma^0(x')dx'\right]\psi_j(x) = \epsilon_j\psi_j(x). \tag{2.25}$$

The states $|i\rangle$ and $|f\rangle$ in this case are identical determinants built of ψ_j, and the zeroth order stationary-phase evolution operator becomes[1]

$$\langle i|U(t_f,t_i)|i\rangle \approx \exp\left(\tfrac{1}{2}i\int\int\int\sigma^0 V\sigma^0\right)\exp\left[-i(t_f-t_i)\sum_j\epsilon_j\right]$$
$$= \exp\left\{-i\left[\sum_j\left\langle j\left|\frac{p^2}{2m} - \tfrac{1}{2}V(0)\right|j\right\rangle + \tfrac{1}{2}\sum_{jk}\langle jk|V|jk\rangle\right](t_f-t_i)\right\}, \tag{2.26}$$

where $|j\rangle$ denotes the single-particle eigenfunction ψ_j. The total phase of $\langle i|U|i\rangle$ evolves with the Hartree energy, including the proper factor of $\frac{1}{2}$, plus the extra self-energy term $-\frac{1}{2}V(0)$.

For such stationary solutions, the quadratic corrections (2.23) simplify considerably. The expression (2.21) for D_0 reduces to the density correlation function of the noninteracting system in the potential $\int V(x-x')\sigma^0(x')dx'$,

$$iD_0^{\text{static}}(xt;x't) \equiv iD_0^{\text{static}}(x,x')$$
$$= \rho(x)\delta(x-x') - \rho(x,x')\rho(x',x) \tag{2.27}$$

where the one-body density matrix is defined as

$$\rho(x', x) \equiv \sum_{j=1}^{A} \psi_j^*(x)\psi_j(x') . \tag{2.28}$$

With this result for D_0^{static} the first term in the sum over n in Eq. (2.23) yields the leading order correction

$$\begin{aligned}\tfrac{1}{2}\,\mathrm{tr}D_0(V\delta) &= \tfrac{1}{2}\int dx\,dx'dt\,D_0^{\text{static}}(xt;x't)V(x-x') \\ &= -\tfrac{1}{2}i\int dx\,dx'dt[\rho(x)\delta(x-x') \\ &\quad -\rho(x,x')\rho(x',x)]V(x-x') \\ &= -i\left[\frac{NV(0)}{2} - \tfrac{1}{2}\sum_{jk}\langle jk\,|\,V\,|kj\rangle\right](t_f - t_i) .\end{aligned} \tag{2.29}$$

This leading correction to the phase of Eq. (2.26) modifies the expression for the energy in a remarkable way. The first term of (2.29) precisely cancels the unpleasant self-energy term whereas the second term inserts the proper exchange matrix elements. Although the single-particle basis $\{\psi_j\}$ is determined by the solution of (2.25) which includes the unphysical self-energy and only the Hartree potential, at least the energy is evaluated using the more physical Hartree-Fock expression in this nonoptimal basis.

The sum over $n > 1$ in (2.23) is easily understood by noting that the product $D_0(V\delta)$ is just a closed particle-hole fermion loop connected to an instantaneous potential interaction, so that $[D_0(V\delta)]^n$ generates an n term RPA chain of particle-hole excitations connected by direct matrix elements. The trace simply connects the chain back on itself, creating an RPA ring and the $1/n$ corrects for the n different ways one could pick the top of the ring. The summation over n thus includes exactly all direct RPA diagrams with no overcounting of the second-order term. That the counting is correct may also be checked from the familiar Green's function formula[5] for a homogeneous system for the energy per unit volume

$$\begin{aligned}\frac{E_{\text{RPA}}}{\Omega} &= \tfrac{1}{2}i\int\frac{d^3q\,d\omega}{(2\pi)^4}\int_0^1\frac{d\lambda}{\lambda}\frac{[\lambda V(q)D_0(q,\omega)]^2}{1-\lambda V(q)D_0(q,\omega)} \\ &= \tfrac{1}{2}i\int\frac{d^3q\,d\omega}{(2\pi)^4}\sum_{n=2}^{\infty}\frac{1}{n}[D_0(q,\omega)V(q)]^n ,\end{aligned} \tag{2.30}$$

where $D_0(q,\omega)$ and $V(q)$ are the Fourier transforms of $D_0(x-x';t-t')$ and $V(x-x')\delta(t-t')$, respectively.

In summary, all the quadratic corrections bring the stationary-phase evolution operator in the static case to the form

$$\langle i\,|\,U(t_f,t_i)\,|\,i\rangle \simeq \exp\left\{-i\left[\sum_j\left\langle j\left|\frac{p^2}{2m}\right|j\right\rangle + \tfrac{1}{2}\sum_{k,j}\langle kj|\,V\,|kj-jk\rangle + E_{\text{RPA}}\right](t_f-t_i)\right\} . \tag{2.31}$$

The changes relative to Eq. (2.26) are twofold. By (2.29), the leading quadratic correction cancels the self-energy

$$-\tfrac{1}{2}\sum_{j=1}^{A}\langle j\,|\,V(0)\,|j\rangle$$

and inserts the exchange term $-\sum_{jk}\langle jk\,|\,V\,|kj\rangle$. Also, by Eq. (2.30), the sum of all higher order corrections includes the direct RPA ring diagrams.

The corrected Hartree result, Eq. (2.31), permits a consistency check of our stationary-phase approach in a special case for which it should yield a known asymptotic result. For the case of a one dimensional system of N fermions with spin $2S+1 > N$ interacting via an attractive delta-function potential, the ground-state energy of the N-particle bound state has a $1/N$ expansion.[6] Specifically, the contribution of any Goldstone diagram with I interactions and C closed fermion loops is of order N^{C-I+2}. Thus, the direct Hartree energy, with two loops and one interaction is of order N^3 and the only diagrams of order N^2 are the exchange Fock term and all the direct RPA ring diagrams. In the present treatment, since S_{eff} is proportional to N, one expects application of the stationary-phase approximation to yield an asymptotic expansion in $1/N$. The leading term is the expected Hartree result, plus the annoying singular constant self-energy term $V(0)$. The quadratic corrections are supposed to pick up all terms of next order in $1/N$, and indeed they do reproduce the exchange term and direct RPA diagrams as well as removing the troublesome self-energy. Thus, in this simple case where an asymptotic expansion is already known, it is verified that the functional integral technique is working quite satisfactorily.

C. Nonlocal mean fields

The essential lesson from the last section is that there is nothing intrinsically unsatisfactory about successive functional integral approximations generated by corrections to the stationary-

phase approximation. Statistics ultimately are properly included and the self-energy term is eliminated by the leading order quadratic correction. However, from a practical point of view, it is quite unsatisfactory to be forced to deal with a first approximation generated by the Hartree potential plus self-energy terms. For static nuclear problems, even after taking care of the hard core, the Hartree potential contributes less than half of the potential energy, so nuclei would not even be bound in this approximation.

The origin of the Hartree mean field in this formulation is evident from Eqs. (2.2) and (2.6). The mean field σ^0 in Eq. (2.13) cannot escape being local because the Hamiltonian has been expressed solely in terms of $\hat{\rho}(x)$. Since considerable freedom exists in how one chooses to express the second quantized two-body interaction operator, it will be useful to consider the following general expression for the interaction term:

$$V=\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\psi_\alpha^\dagger\psi_\beta^\dagger V_{\alpha\beta\gamma\delta}\psi_\delta\psi_\gamma$$
$$=\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\hat{\rho}_{\alpha\gamma}V_{\alpha\beta\gamma\delta}\hat{\rho}_{\beta\delta}-\tfrac{1}{2}\sum_{\alpha\beta\delta}\hat{\rho}_{\alpha\delta}V_{\alpha\beta\beta\delta}\,, \qquad (2.32)$$

where

$$\hat{\rho}_{\alpha\gamma}\equiv\psi_\alpha^\dagger\psi_\gamma$$

and the indices $\alpha\beta\gamma\delta$ are used to denote an arbitrary single-particle representation. Repetition of the previous derivation simply replaces the former local density operator $\hat{\rho}(x)$ by the nonlocal operator $\hat{\rho}_{\alpha\beta}$. The functional integral (2.6) is replaced by an integral over a nonlocal $\sigma_{\alpha\beta}(t)$ so that the stationary-phase result (2.17) is replaced by

$$\sigma^0_{\alpha\beta}(t)=\langle\Phi(t)\,|\,\hat{\rho}_{\alpha\beta}(t)\,|\,\Phi(t)\rangle\,. \qquad (2.33)$$

In coordinate representation, it is crucial to bear in mind that α denotes spin and isospin projections $s_\alpha\tau_\alpha$ as well as the spatial variable x_α, so that

$$\sigma^0_{\alpha\beta}(t)\equiv\sigma^0_{\alpha\beta}(x_\alpha,x_\beta,t)$$
$$=\delta_{s_\alpha s_\beta}\delta_{\tau_\alpha\tau_\beta}\sum_{j=1}^{A}\phi^*_{js_\alpha\tau_\alpha}(x_\alpha,t)\phi_{js_\beta\tau_\beta}(x_\beta,t)\,. \qquad (2.34)$$

The evolution operator U_{t0} then evolves single-particle wave functions according to the one-body operator h

$$i\dot{\psi}_\beta=\sum_\delta h_{\beta\delta}\psi_\delta\,, \qquad (2.35)$$

where

$$h_{\beta\delta}=\left(T_{\beta\delta}-\sum_\alpha\tfrac{1}{2}V_{\beta\alpha\alpha\delta}+\sum_{\alpha\gamma}\sigma_{\alpha\gamma}V_{\alpha\beta\gamma\delta}\right)\hat{\rho}_{\beta\delta} \qquad (2.36)$$

and $T_{\beta\delta}$ is the kinetic energy matrix element. Similarly, second variation of the effective action replaces Eq. (2.22) by the result

$$\frac{\delta^2 S_{\rm eff}}{\delta\sigma_{\alpha\gamma}(t)\delta\sigma_{\alpha'\gamma'}(t')}=\int dt''\sum_{\beta\delta}V_{\alpha\beta\gamma\delta}\delta(t-t'')$$
$$\times\left[\delta(t''-t')\delta_{\beta\alpha'}\delta_{\delta\gamma'}-\int dt'''\sum_{\beta'\delta'}\delta(t'''-t')V_{\alpha'\beta'\gamma'\delta'}D^0_{\beta\delta\beta'\delta'}(t'',t''')\right], \qquad (2.37)$$

where

$$iD^0_{\beta\delta\beta'\delta'}(t'',t''')=\langle\langle\hat{\rho}_{\beta\delta}(t'')\hat{\rho}_{\beta'\delta'}(t''')\rangle\rangle-\langle\langle\hat{\rho}_{\beta\delta}(t'')\rangle\rangle\langle\langle\hat{\rho}_{\beta'\delta'}(t''')\rangle\rangle \qquad (2.38)$$

and

$$\langle\langle O\rangle\rangle\equiv\frac{\langle f\,|\,\tau O\exp(-i\sum_{\alpha\beta\gamma\delta}\int\sigma^0_{\alpha\gamma}(t)V_{\alpha\beta\gamma\delta}\hat{\rho}_{\beta\delta}(t))\,|\,i\rangle}{\langle f\,|\,\tau\exp(-i\sum_{\alpha\beta\gamma\delta}\int\sigma^0_{\alpha\gamma}(t)V_{\alpha\beta\gamma\delta}\hat{\rho}_{\beta\delta}(t))\,|\,i\rangle}\,. \qquad (2.39)$$

The leading order quadratic correction is again given by the trace of $(V\delta)D^0$, and in the static case yields

$$\tfrac{1}{2}\mathrm{tr}\,[(V\delta)D_0]=-\tfrac{1}{2}i\int_{t_i}^{t_f}dt\sum_{\beta\beta'\delta\delta'}V_{\beta\beta'\delta\delta'}\{\langle\Phi\,|\,\hat{\rho}_{\beta\delta}\hat{\rho}_{\beta'\delta'}\,|\,\Phi\rangle-\langle\Phi\,|\,\rho_{\beta\delta}\,|\,\Phi\rangle\langle\Phi\,|\,\rho_{\beta'\delta'}\,|\,\Phi\rangle\}$$
$$=-\tfrac{1}{2}i\left\{\sum_{\beta\gamma\delta'}V_{\beta\gamma\gamma\delta'}\langle\rho_{\beta\delta'}\rangle-\sum_{\beta\beta'\delta\delta'}V_{\beta\beta'\delta\delta'}\langle\rho_{\beta'\delta}\rangle\langle\rho_{\beta\delta'}\rangle\right\}(t_f-t_i)\,, \qquad (2.40)$$

with the notation $\langle\rho\rangle=\langle\Phi\,|\,\hat{\rho}\,|\,\Phi\rangle$.

With the results of Eqs. (2.33) through (2.40), it is now straightforward to explore nonlocal mean fields. Because (2.32) is manifestly antisymmetric, we are free to replace $V_{\alpha\beta\gamma\delta}$ by $-V_{\alpha\beta\delta\gamma}$. The previous Hartree results for a central potential are recovered by the choice

$$V_{\alpha\beta\gamma\delta}=\delta(x_\alpha-x_\gamma)\delta_{s_\alpha s_\gamma}\delta_{\tau_\alpha\tau_\gamma}\delta(x_\beta-x_\delta)\delta_{s_\beta s_\delta}\delta_{\tau_\beta\tau_\delta}V(x_\alpha-x_\beta)\,. \qquad (2.41)$$

The mean field in Eq. (2.36) is rendered local by the factor $\delta(x_\beta - x_\delta)$ and depends only on the local density $\rho_{\alpha\alpha}$. The first term in the leading quadratic correction, Eq. (2.40), is a self-energy term which exactly cancels that in (2.36) and the remaining correction is the familiar exchange term to the energy

$$-\tfrac{1}{2}\int dx \int dx' V(x-x') \sum_{\substack{mm' \\ s\tau}} \psi^*_{ms\tau}(x)\psi_{ms\tau}(x')\psi^*_{m's\tau}(x')\psi_{m's\tau}(x) . \tag{2.42}$$

Using the equally valid expression for a central potential

$$V_{\alpha\beta\gamma\delta} = -\delta(x_\alpha - x_\delta)\delta_{s_\alpha s_\delta}\delta_{\tau_\alpha\tau_\delta}\delta(x_\beta - x_\gamma)\delta_{s_\beta s_\gamma}\delta_{\tau_\beta\tau_\gamma} V(x_\alpha - x_\beta) \tag{2.43}$$

yields a mean field with no Hartree term and precisely the Fock exchange term. Explicitly, the mean-field term in (2.36) yields

$$h(x;x)_{s\tau s'\tau'} = -V(x-x') \sum_{ms''\tau''} \psi^*_{ms''\tau''}(x)\psi_{ms''\tau''}(x')\delta_{ss'}\delta_{\tau\tau'} . \tag{2.44}$$

Although this Fock mean-field result is *a priori* as unsatisfying as the Hartree result, the leading second-order correction again yields just the Hartree-Fock energy expression. As before, the self-energy terms in (2.36) and (2.40) exactly cancel. The overall $\frac{1}{2}\int\int\int \sigma^0 V \sigma^0$ factor removes half the exchange term so it is counted correctly. Finally, substitution of (2.43) into the last term of (2.40) produces the direct Hartree term. Thus, the two exact expressions (2.41) and (2.43) yield very different mean fields but the same leading order corrected energy expressions to be evaluated using the respective Hartree or Fock wave functions.

At this point, it is suggestive to consider the connection between the artificial σ field and the actual meson fields present if there were an underlying field theory. In the case of a field theory of fermions and mesons, our stationary field σ^0 corresponds to the meson field generated by the self-consistent distribution of fermions and the RPA quadratic corrections correspond to the one-meson loop corrections in field theory. Since scalar and vector meson couplings single out direct and exchange matrix elements, respectively, one can construct a model system in which Hartree and Fock terms arise from scalar and vector components of the model, respectively. In the same $1/N$ limit discussed previously, such a model yields an exact Hartree-Fock theory.

The feature of the field theory model that different components lead naturally to direct and exchange terms suggests that one consider decomposing the static two-body potential V in the nonrelativistic problem into two distinct components: one which will generate the Hartree potential and another which will generate the exchange potentials. At the level of a pure one-boson-exchange potential this decomposition follows from the previous arguments; for example, the one-pion-exchange potential contributes to the HF energy of nuclear matter only through the exchange term. For a general phenomenological potential, we must relinquish the formal connection with vector or scalar exchanges, and simply explore the possible advantage of decomposing the potential into two parts which are subsequently treated differently.

To render the decomposition well defined, physically motivated, and in some sense optimal, it is desirable to require that the leading quadratic correction to the energy vanish. Thus, the freedom in specification of the mean field is utilized to improve the accuracy of the stationary-phase approximation. The basic strategy is to decompose the interaction as follows:

$$\begin{aligned} V_{\alpha\beta\gamma\delta} &\equiv V^{(D)}_{\alpha\beta\gamma\delta} + V^{(E)}_{\alpha\beta\gamma\delta} \\ &= V^{(D)}_{\alpha\beta\gamma\delta} - V^{(E)}_{\alpha\beta\delta\gamma} , \end{aligned} \tag{2.45}$$

such that the Fock term of $V^{(D)}$ and the Hartree term of $V^{(E)}$ vanish. It is particularly convenient to accomplish this decomposition via spin algebra, since the self-energy terms are easily eliminated at the same time. For closed-shell nuclei, nuclei with at most one particle or hole relative to a closed shell, or any nuclei treated in the filling approximation, both terms in Eq. (2.40) necessarily involve the spin sum $\sum_{ss'} V_{ss's's}$, where either s or s' is summed over a closed shell. Hence, for these cases, we may require that the following spin sums vanish:

$$\sum_s V^{(D)}_{ss's's} = \sum_s V^{(E)}_{ss'ss'} = 0 . \tag{2.46}$$

This condition is straightforward to implement using the spin exchange operator P_s by noting that

$$\sum_s \langle ss' | 1 - \tfrac{1}{2}P_s | s's\rangle = \sum_s \langle ss' | 1 - 2P_s | ss'\rangle = 0 . \tag{2.47}$$

For a central, spin-dependent potential

$$V + V_s P_s = V^{(D)} + V^{(E)} , \tag{2.48}$$

where

$$V^{(D)} = \tfrac{1}{3}(2 - P_s)(2V + V_s)\,,$$
$$V^{(E)} = -\tfrac{1}{3}(1 - 2P_s)(V + 2V_s)\,. \tag{2.49}$$

For a nuclear potential defined in the singlet-even, triplet-even, singlet-odd, and triplet-odd channels,

$$V^D = \tfrac{1}{12}(2 - P_s)[(V^{\mathrm{SE}} + 3V^{\mathrm{TE}} + V^{\mathrm{SO}} + 3V^{\mathrm{TO}}) + (V^{\mathrm{SE}} - 3V^{\mathrm{TE}} - V^{\mathrm{SO}} + 3V^{\mathrm{TO}})P_\tau]$$
$$V^E = -\tfrac{1}{12}(1 - 2P_s)[(-V^{\mathrm{SE}} + 3V^{\mathrm{TE}} - V^{\mathrm{SO}} + 3V^{\mathrm{TO}}) + (-V^{\mathrm{SE}} - 3V^{\mathrm{TE}} + V^{\mathrm{SO}} + 3V^{\mathrm{TO}})P_\tau]\,. \tag{2.50}$$

It may be verified by straightforward algebra that (2.49) or (2.50) yields precisely the usual Hartree-Fock equations[7] when $V^D_{\alpha\beta\gamma\delta} - V^E_{\alpha\beta\delta\gamma}$ is substituted into Eqs. (2.35) and (2.36). Thus, the decomposition (2.45) of the interaction which was devised to make the leading quadratic correction vanish leads to the Hartree-Fock equations for the single-particle basis. This basis may, therefore, be considered as optimal with regard to the improvement of the accuracy of the stationary-phase approximation.

The full flexibility of the Hubbard-Stratonovich transformation to define alternative mean fields has still not been fully utilized. As noted by Hubbard,[4] one could introduce a complex field $\sigma(x, x')$ and obtain the result[16]

$$\tau \exp\left[-\tfrac{1}{2}i \int dx\,dx'\,dt\,\eta^\dagger(x, x't)V(x - x')\eta(x, x't)\right] = \int D[\sigma] \exp\left[\tfrac{1}{2}i \int dx\,dx'\,dt\,\sigma^*(x, x't)V(x - x')\sigma(x, x't)\right] \times \tau \exp\left\{-\tfrac{1}{2}i \int V(x - x')[\sigma^*(x, x', t)\eta(x, x', t) + \sigma(x, x', t)\eta^\dagger(x, x', t)]\right\}, \tag{2.51}$$

where

$$\eta(x, x') = \psi(x)\psi(x')\,. \tag{2.52}$$

The mean field in this case is the pairing field

$$\sigma(x, x', t) = \frac{\langle f|U_\sigma(t_f, t)\psi(x)\psi(x')U_\sigma(t, t_i)|i\rangle}{\langle f|U_\sigma(t_f, t_i)|i\rangle}\,. \tag{2.53}$$

Although (2.53) is nonvanishing for determinantal wave functions because U_σ violates number conservation, it appears more natural in this case to use BCS wave functions in which case σ is just the usual BCS order parameter Δ. Presumably, a suitable decomposition of the interaction exists such that the stationary-phase approximation yields the time-dependent Hartree-Fock-Bogoliubov equation, but we have not explicitly constructed it. Quadratic corrections to the stationary-phase approximation will differ from the previous case only in that D^0 will contain particle-particle and hole-hole bubbles rather than particle-hole bubbles. The analog of the RPA sum is thus Brueckner ladder diagrams and analogous down going ladders.

The main conclusion of this section is that it is indeed possible to obtain time-dependent Hartree-Fock equations in the stationary-phase approximation. Of all the arbitrary ways of decomposing the interaction, this particular choice has the specific advantage of having no first-order quadratic corrections to the energy. Having demonstrated that the local Hartree equations can always be straightforwardly generalized to a corresponding Hartree-Fock theory, for pedagogical clarity and economy of notation, we will henceforth only write out the special Hartree limit.

III. QUANTIZED BOUND STATES

In this chapter we evaluate the bound state spectrum using a method suggested by Gutzwiller[8] and exploited extensively in the semiclassical analysis of field theory.[2] To relate our approximation of the evolution operator, $U(T, O) = e^{-iHT}$ to the eigenvalues, E_ν of H, it is convenient to use the identity

$$G(E) \equiv i \int_0^\infty dT e^{iET}\,\mathrm{tr}U(T, O) = \sum_\nu \frac{1}{E_\nu - E}\,, \tag{3.1}$$

where E is defined to have a small positive imaginary part to ensure convergence, periodic boundary conditions are assumed to render the spectrum discrete, and the trace is evaluated in the space of antisymmetric A-particle wave functions. In this section, we will obtain approximate eigenvalues by examining the poles of $G(E)$ in lowest order SPA, and discussion of higher corrections is deferred to Sec. V. In many respects our treatment follows that of the Gross-Neveu model by Dashen, Hasslacher, and Neveu.[2] However, we avoid problems related to integration over anticommuting c-number variables and use a language

appropriate to nuclear physics.

By (2.6), the quantity $\mathrm{tr}U(T,O)$ appearing in (3.1) may be rewritten

$$\mathrm{tr}U(T,O)=\int D[\sigma]\exp\left(\tfrac{1}{2}i\int\sigma V\sigma\right)\mathrm{tr}U_\sigma(T,O)\,, \tag{3.2}$$

where in Schrödinger representation

$$U_\sigma(T,O) =\tau\exp\left\{-i\int_0^T dt\left[K+\int\int dx\,dx'\hat{\rho}(x)\times V(x-x')\sigma(x',t)\right]\right\}. \tag{3.3}$$

The trace of U_σ is conveniently evaluated in the basis of its eigenfunctions. Since U_σ describes the time evolution in a one-body potential, it may be written as a product of A formally identical single-particle evolution operators

$$U_\sigma^{(s.p.)}=\tau\exp\left[-i\int_0^T h_\sigma(t)dt\right], \tag{3.3a}$$

where $h_\sigma(t)$ is

$$h_\sigma(t)=\frac{p^2}{2m}-\tfrac{1}{2}V(0)+\int V(x-x')\sigma(x',t)dx'\,. \tag{3.3b}$$

The eigenfunctions of $U_\sigma^{(s.p.)}$ satisfy

$$U_\sigma^{(s.p.)}(T,O)\,|\phi_j\rangle=e^{-i\alpha_j}|\phi_j\rangle\,, \tag{3.4}$$

where the $\alpha_j=\alpha_j[\sigma]$ are real by unitarity. The antisymmetrized eigenfunctions of U_σ are generated by the set of solutions of (3.4) and thus the trace may be written

$$\mathrm{tr}U_\sigma(T,O)=\sum_{\{n\}}\exp\left(-i\sum_{j=1}^{\infty}n_j\alpha_j[\sigma]\right), \tag{3.5a}$$

where $\{n\}$ denotes all possible sets of fermion occupation numbers in the basis $|\phi_j\rangle$

$$n_j=0 \text{ or } 1\,,\quad \sum_{j=1}^{\infty}n_j=A\,. \tag{3.5b}$$

To calculate the eigenvalues α_j, it is convenient to cast Eq. (3.4) into differential form, by defining

$$|\phi_j(t)\rangle\equiv U_\sigma^{(s.p.)}(t,0)\,|\phi_j\rangle\,.$$

These single-particle functions satisfy the Schrödinger equation with the time-dependent Hamiltonian (3.3b)

$$\left(i\frac{\partial}{\partial t}-h_\sigma(t)\right)|\phi_j\rangle=0\,, \tag{3.6a}$$

subject to the boundary condition

$$|\phi_j(T)\rangle=e^{-i\alpha_j}|\phi_j(0)\rangle\,. \tag{3.6b}$$

Equations (3.6) may be rewritten as a differential eigenvalue problem by defining the wave functions

$$|u_j(t)\rangle=e^{i\alpha_j t/T}|\phi_j(t)\rangle\,, \tag{3.7}$$

which satisfy

$$\Lambda_\sigma|u_j\rangle\equiv\left(i\frac{\partial}{\partial t}-h_\sigma\right)|u_j\rangle=-(\alpha_j/T)\,|u_j\rangle \tag{3.8a}$$

and the periodic boundary condition

$$|u(T)\rangle=|u(0)\rangle\,. \tag{3.8b}$$

The operator Λ_σ is Hermitian in the Hilbert space of functions satisfying (3.8b) where integration over all space and the time interval $0<t<T$ is implied in all inner products. Since the σ's of subsequent interest will be periodic in time T, $\sigma(t)=\sigma(t+T)$, the solutions of (3.6a) are Bloch waves in the time variable t and Eq. (3.6b) is the counterpart of Bloch's theorem. In analogy with quasimomentum in a spatially periodic potential, the quantity α_j/T can be regarded as a quasienergy in the case of periodicity in time. In the special limit of a time-independent σ,

$$\alpha_j=\epsilon_j T\,, \tag{3.9}$$

where ϵ_j denotes an eigenvalue of the single-particle Hamiltonian h_σ.

Substitution of (3.5a) into Eq. (3.2) yields

$$\mathrm{tr}U(T,O)=\sum_{\{n\}}\int D[\sigma]\exp\left(\tfrac{1}{2}i\int\sigma V\sigma-i\sum_{j=1}^{\infty}n_j\alpha_j[\sigma]\right). \tag{3.10}$$

A. The periodic mean field

Equation (3.10) is now cast in a form in which one can single out of the infinite set of σ's required to evaluate $\mathrm{tr}U$ exactly a small number of stationary-phase solutions. However, it is still necessary to choose whether to apply the SPA to each term in the sum over $\{n\}$ separately, to subgroups of terms, or to the entire sum. In this present work, we choose to treat each set of occupation numbers separately, both because we believe this is the most physical choice for discrete bound state energies and because of the technical simplification arising from a formulation based on a single determinant. For other applications, such as evaluating a suitably averaged density of states in the continuum, application of SPA to the whole sum may be preferable. In the next section, in the context of a simple model we will discuss the results of other possible choices.

In applying SPA to a particular term of (3.10) we solve for those σ which satisfy

$$\delta S[\sigma]=0, \tag{3.11}$$

where

$$S[\sigma]=\tfrac{1}{2}\int \sigma V\sigma-\sum_{j=1}^{\infty} n_j\alpha_j[\sigma]. \tag{3.12}$$

To evaluate δS it is necessary to find the variation of α_j when σ is varied. From (3.8) we obtain using first-order perturbation theory

$$\frac{\delta\alpha_j}{T}=\frac{\int_0^T dt\int dx u_j^*(x,t)\delta\Lambda_\sigma u_j(x,t)}{\int_0^T dt\int dx\,|u_j(x,t)|^2}, \tag{3.13a}$$

with

$$\delta\Lambda_\sigma=\int dx' V(x-x')\delta\sigma(x',t)dx'. \tag{3.13b}$$

Hermiticity of h_σ in its spatial variables implies that the integral over x in the denominator of (3.13a) is time independent and we may normalize $u_j(x,t)$ to unity:

$$\int |u_j(x,t)|^2dx=\int |\phi_j(x,t)|^2dx=1. \tag{3.13c}$$

The stationary-phase condition (3.11) is now

$$\delta S=\int \delta\sigma V\sigma-\sum_{j=1}^{\infty} n_j\int \delta\sigma V|\phi_j|^2=0$$

with the solution

$$\sigma^0(x,t)\equiv\rho(x,t)=\sum_{j=1}^{\infty} n_j|\phi_j(x,t)|^2. \tag{3.14}$$

In the lowest order SPA Eq. (3.10) becomes

$$\mathrm{tr}U(T,O)\approx\sum_{\sigma^0} e^{iS[\sigma^0,T]}, \tag{3.15}$$

where the sum is taken over all different solutions σ^0 of Eq. (3.14) for all possible sets of $\{n\}$. The result (3.15) is valid only when all the stationary points of S are well separated. Otherwise, a more careful treatment including the second variation $\delta^2S/\delta\sigma\delta\sigma$ is required. One possible problem is the occurrence of zero eigenvalues of $\delta^2S/\delta\sigma\delta\sigma$ due to continuous symmetries of the exact problem which are broke by σ^0. This possibility may be treated by the general methods of Ref. 9, and usually leads to obvious corrections, such as the center of mass motion in the case of translational symmetry. Although we did not perform a detailed evaluation, we do not expect that it will affect the subsequent presentation. Another possibility is related to the so-called dynamical zero eigenvalues of $\delta^2S/\delta\sigma\delta\sigma$ when some of the stationary points of S occasionally coalesce. In this event a more complicated uniform expression[10] should replace (3.15). We will not discuss such cases here.

The mean field σ^0 and the eigenvalues $\alpha_k[\sigma^0]$ are found by solving Eq. (3.6) with σ satisfying the condition (3.14). When this self-consistency condition is introduced into Eq. (3.6a) the latter acquires a familiar time-dependent Hartree form. In the previous section we demonstrated how to generalize this equation by including the exchange potential and removing the self-energy term $-\frac{1}{2}V(0)$. For the sake of notational simplicity, we will continue to write only the Hartree term, but we will subsequently refer to Eq. (3.6a) with the self-consistent σ as the TDHF equation.

The boundary condition (3.6b) represents a crucial new element in the present formulation of the time-dependent mean-field theory. Because of this condition, the mean-field potential $\int V(x-x')\times\sigma^0(x';t)dx'$ is periodic in time and as discussed earlier, the eigenvalues α_j/T are quasienergies in this self-consistent potential. One therefore has a time-dependent generalization of the conventional static HF problem, which is most explicit in the eigenvalue form (3.8). The time-dependent operator Λ_σ with $\sigma=\sigma^0$ replaces the static HF Hamiltonian h_{σ^0} and the periodicity condition (3.8b) on the time variable is added to the appropriate spatial boundary conditions. The static HF equations appear as a particular case of (3.8a) with time-independent σ^0.

The HF energy

$$\begin{aligned}E_{\mathrm{HF}}(T)&=\sum_{k=1}^{A}\langle\phi_k|h_{\sigma^0}|\phi_k\rangle-\tfrac{1}{2}\int\int dx\,dx'\sigma^0V\sigma^0\\&=\frac{1}{2m}\sum_{k=1}^{A}\int dx|\nabla\phi_k|^2\\&\quad+\tfrac{1}{2}\sum_{k,j=1}^{A}\int\int|\phi_k|^2V|\phi_j|^2dx\,dx'-\tfrac{1}{2}AV(0)\end{aligned} \tag{3.16}$$

is conserved by the TDHF equations, where, for convenience, we have assumed that the occupation numbers are labeled such that $n_j=1$ for $j\leq A$ and zero otherwise. In contrast to the usual TDHF initial value problem in which E_{HF} is specified by the initial wave function, in the present theory E_{HF} is specified by the self-consistent solution of Eq. (3.6) and in general is determined by the period T.

Only in the static case when

$$\phi_k(x,t)=\psi_k(x)e^{-i\epsilon_k t} \tag{3.17}$$

is the value of E_{HF} independent of T. The implicit T dependence of Eq. (3.16) will be important in the next section in calculating quantized states.

B. Quantization condition

The final step in calculating $G(E)$ is evaluation of the time integral. Substitution of the SPA result (3.15) in Eq. (3.1) yields

$$G(E) \simeq i\sum_{\sigma^0}\int_0^\infty dT\, e^{i(ET+S[\sigma^0,T])}, \tag{3.18}$$

the poles of which approximate the energy eigenvalues of the system.

For the special case of time-independent σ^0, we expect to recover the static HF energy. This expectation is verified by evaluating $S[\sigma^0, T]$ using Eqs. (3.12) and (3.9):

$$S[\sigma^0, T]=\left(\tfrac{1}{2}\int dx\, dx'\sigma^0(x)V(x-x')\sigma^0(x') - \sum_{j=1}^{\infty} n_j\epsilon_j\right)T$$

$$=-E_{\mathrm{HF}}^{\mathrm{static}}\, T, \tag{3.19}$$

where $E_{\mathrm{HF}}^{\mathrm{static}}$ represents the HF energy (3.16) for the static wave functions (3.17) with occupation numbers $\{n\}$. The linear T dependence in (3.19) immediately implies a pole in $G(E)$, Eq. (3.18), at E_{HF}, so that static HF energies for all distinct sets of occupation numbers are recovered.

More interesting states arise from consideration of a time-dependent σ^0. Owing to the nontrivial dependence of S on T in this case, we apply the SPA to the time integral (3.18). The stationary-phase condition is

$$\frac{\partial}{\partial T}(ET+S[\sigma^0, T]) = E+\frac{\partial S}{\partial T}=0. \tag{3.20}$$

Using the explicit expression (3.12) for S we derive in Appendix B the intuitively expected result

$$\frac{\partial S}{\partial T}=-E_{\mathrm{HF}}(T), \tag{3.21}$$

where $E_{\mathrm{HF}}(T)$ is the HF energy (3.16) of the time-dependent solution of (3.6) with $\sigma=\sigma^0$.

The SPA condition (3.20) thus implicitly defines values of T for which

$$E=E_{\mathrm{HF}}(T). \tag{3.22}$$

In the lowest order of SPA a given solution $T^0(E)$ of this equation contributes a term

$$\exp\{i[E_{\mathrm{HF}}(T^0)T^0+S[\sigma^0, T^0]]\}$$

to $G(E)$. Owing to the periodicity of the time-dependent σ^0, any integral multiple of T_0 is also a solution of (3.22) since $E_{\mathrm{HF}}(kT^0)=E_{\mathrm{HF}}(T^0)$. The quasienergies α_j for such multiple cycle are

$$\alpha_j[kT^0]=k\alpha_j[T^0]$$

and the corresponding action satisfies

$$S[\sigma^0, kT^0]=kS[\sigma^0, T^0].$$

Each multicycle stationary solution contributes to $G(E)$ in the SPA generating the geometric series

$$\sum_{k=1}^{\infty} e^{ikW(E)}=\frac{e^{iW(E)}}{1-e^{iW(E)}}, \tag{3.23}$$

where

$$W(E)=E_{\mathrm{HF}}T^0+S[\sigma^0, T^0] \tag{3.24}$$

and $T^0(E)$ denotes the basic (smallest) period of the σ^0 which satisfies (3.22).

The periodic time-dependent σ^0 produces a pole in $G(E)$ at values of $E=E_{\mathrm{HF}}$ when

$$W(E)=2m\pi, \quad m \text{ integer}. \tag{3.25}$$

The value of this energy gives an approximation to a bound state of the nuclear system corresponding to a dynamic periodic motion of the self-consistent mean field σ^0.

Before discussing this result further it will be useful to summarize the steps and equations for the calculation of these periodic solutions.

One starts from the TDHF equations

$$i\dot{\phi}_j=\left(\frac{p^2}{2m}-\tfrac{1}{2}V(0)+\int V(x-x')\right.$$

$$\left.\times\sum_{k=1}^{A}|\phi_k(x', t)|^2dx'\right)\phi_j \tag{3.26a}$$

and finds the solution which for a given time interval T satisfies the condition

$$\phi_j(x, t)=e^{-i\alpha_j}\phi_j(x, 0), \quad j=1, \ldots, A. \tag{3.26b}$$

The HF energy of this solution $E_{\mathrm{HF}}(T)$ depends on the time interval T, and one must finally find the value of T for which the condition (3.25) is satisfied. The resulting value of E_{HF} then gives the approximate energy level of the system.

The function $W(E)$ may be expressed in terms of the solution of (3.26) by substituting

$$E_{\mathrm{HF}}T^0=-\tfrac{1}{2}\int_0^{T^0}dt\int dx\, dx'\sigma^0V\sigma^0$$

$$+\sum_{k=1}^{A}\int_0^{T^0}dt\langle\phi_k|h_{\sigma^0}|\phi_k\rangle \tag{3.27}$$

and Eq. (3.12) into (3.24).

Using Eq. (3.6a) to replace $\langle\phi_k|h_{\sigma^0}|\phi_k\rangle$ by $\langle\phi_k|i\partial/\partial t|\phi_k\rangle$ yields

$$\sum_{k=1}^{A}\left[\int_0^{T^0}dt\int dx i\phi_k^*(x, t)\frac{\partial\phi_k}{\partial t}(x, t)-\alpha_k\right]=2m\pi. \tag{3.28}$$

The first term in (3.28) has a simple physical meaning if one adopts the interpretation of the TDHF equations as equations for coupled classical fields.[11] In this interpretation ϕ_k and $i\phi_k^*$ at each space point are canonically conjugate coordinates and momenta. The first term in (3.28) is therefore of the form $\int p\dot{q}dt$ appearing in the semiclassical Bohr-Sommerfeld quantization rule. Although this form of quantization condition is consistent with the notion that TDHF is in some

sense semiclassical, we find it satisfying that (3.28) has been derived unambiguously without recourse to any philosophy or interpretation.

The presence of the second term in (3.28) containing α_k is important in making the quantization condition invariant under the space independent gauge transformation $\phi_k \to e^{i\chi(t)}\phi_k$. This gauge transformation is equivalent to adding an unobservable c-number term $\dot{\chi}(t)$ to the Hamiltonian and simply adds an overall arbitrary phase. In the following discussion of RPA and the Lipkin model other aspects of the role of the second term in (3.28) will become clear. We note also that using the functions u_j of Eq. (3.7), it is possible to eliminate α_k's from the quantization condition at the expense of introducing them in Eq. (3.8a) for u_j.

Although it is tempting to interpret m in Eq. (3.28) as the number of variational quanta associated with the periodic motion of σ, one must note that α_k is only defined by (3.26b) to within an arbitrary integral multiple of 2π so m has no absolute meaning. In the contexts of the RPA limit and the Lipkin model discussed subsequently, a natural phase convention arises and the physical role of m will be clear. Discussion of the general case is deferred to Sec. V.

Finally, we note that it is useful to consider the eigenvalue form (3.8) of the self-consistent equations (3.26). Because of the mathematical similarity of this self-consistent eigenvalue problem involving the four dimensions x, y, z, t to the well studied static HF problem in three spatial dimensions, one can use the same iterative and numerical methods to obtain the time-dependent self-consistent solutions.

C. The RPA limit

Although the greatest advantage of the preceding quantized nonlinear theory is its applicability to large amplitude collective vibrations, it is instructive to briefly demonstrate that the limit of infinitesimal deviations from the static HF solution reproduces the familiar RPA theory.[12]

Let $\psi_M(x)$ and $\psi_m(x)$ denote the states of a static HF basis where capital and lower case letters denote the A occupied hole states and the set of unoccupied particle states, respectively. A general expansion of the TDHF single-particle wave function in this basis is

$$\phi_K(x,t) = e^{-i\epsilon_K t}\left[\psi_K(x) + \sum_m C_{mK}\psi_m(x)\right] + \sum_M Q_{MK}\psi_M(x) \tag{3.29}$$

and we will assume that the expansion coefficients C_{mK} are small. Since all our previous formulas were written for an orthonormal basis, we must require

$$\int dx\, \phi^*_{K'}(x,t)\phi_K(x,t) = \delta_{KK'}\,, \tag{3.30}$$

which implies

$$\sum_m C^*_{mK'}C_{mK} + \sum_M Q^*_{MK'}Q_{MK} + Q^*_{KK'}e^{-i\epsilon_K t} + Q_{K'K}e^{i\epsilon_{K'}t} = 0\,. \tag{3.31}$$

This condition is satisfied to second order by

$$Q_{MK} = -\tfrac{1}{2}e^{-i\epsilon_M t}\sum_m C^*_{mM}C_{mK} + O(C^3)\,. \tag{3.32}$$

Since Q_{MK} is $O(C^2)$, it may be neglected in the linearized TDHF equations but will be necessary for the energy and quantization conditions.

The usual parametrization

$$C_{mK} = X_{mK}e^{-i\omega t} + Y^*_{mK}e^{i\omega t} \tag{3.33}$$

with time-independent X and Y brings the linearized TDHF equations into a familiar RPA matrix form

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = \omega\begin{pmatrix} X \\ -Y \end{pmatrix}, \tag{3.34}$$

where

$$A_{mM,nN} = (\epsilon_m - \epsilon_M)\delta_{mn}\delta_{MN} + \langle mN|V|Mn\rangle\,, \qquad B_{mM,nN} = \langle mn|V|MN\rangle\,. \tag{3.35}$$

Denoting the RPA eigenvalues and eigenvectors by ω_ν and $(X^{(\nu)}, Y^{(\nu)})$, we now consider application of the periodicity condition (3.26b) to the most general superposition of RPA modes. Except for the special case in which the frequencies of several modes happen to be commensurate, projection of the resulting equation onto the space of unoccupied wave functions requires that only one mode ν be present and that the period satisfy

$$\omega_\nu T_\nu = 2\pi n \tag{3.36}$$

for some integer n. The fundamental period is thus $T_\nu = 2\pi/\omega_\nu$ as expected.

Projection onto each occupied state ψ_k specifies

$$\alpha_K^{(\nu)} = \epsilon_K T_\nu\,. \tag{3.37}$$

As expected for linear vibrations the amplitude which is unspecified by the homogeneous linear RPA equation is determined by the quantization condition (3.28).

By substituting (3.29) into (3.28) and using (3.36), (3.37), and the periodicity of $C^{(\nu)}$, Eq. (3.33), we obtain

$$\int_0^{T_\nu} \sum_{bB} C_{bB}^{(\nu)*} i \frac{\partial}{\partial t} C_{bB}^{(\nu)} = 2m\pi . \tag{3.38}$$

This relation is $O(C^2)$ and it is therefore necessary to include Q_{MK} given by (3.32).

In terms of (X^ν, Y^ν), Eq. (3.38) becomes

$$\sum_{bB} (|X_{bB}^{(\nu)}|^2 - |Y_{bB}^{(\nu)}|^2) = m , \tag{3.39}$$

which is the familiar RPA normalization condition[12] for the m phonon case. The corresponding energy is calculated by substituting (3.29) with (3.32) in (3.16) with the result

$$E_{\mathrm{RPA}}^{(\nu)} = E_{\mathrm{HF}}^{\mathrm{static}} + m\omega_\nu . \tag{3.40}$$

Thus, the general method of the previous section correctly reproduces the RPA limit. Depending on the system under consideration, the amplitudes X and Y may or may not be sufficiently small to justify the linear approximation for low integers in (3.39). Even when the linearity condition is violated, however, the RPA amplitudes may provide a useful starting point for the iterative solution of the full nonlinear problem (3.26).

Several final comments are pertinent to the RPA limit. The arbitrary integer multiple of 2π in the sum $\sum_k \alpha_k$ and the integer in the quantization equation combine to the integer m in Eq. (3.39) which has the physical significance of the number of phonons in the mode ω_ν. The case of zero phonons $m=0$ simply reproduces the static HF solution. The structure of the strict infinitesimal limit is characteristically different from that of the nonlinear theory. One no longer has a continuous family of solutions parametrized by the period T; rather, for $T \neq T_\nu$ there are no periodic solutions and $T = T_\nu$ admits an infinite family of solutions of arbitrary amplitude. The quantization condition is thus decoupled from determination of the period and eigenfunctions and only specifies the allowed amplitudes of the vibrational modes. Considerable insight is obtained by self-consistent numerical solution of a one-dimensional model and will be discussed in a subsequent publication.

IV. APPLICATION TO THE LIPKIN MODEL

A. The model and the associated equations

As a first application, we study the energy levels of an N-fermion system described by the Hamiltonian[13]

$$H = \tfrac{1}{2}\epsilon \sum_{\substack{p=1,2,\ldots,N \\ s=+1,-1}} s a_{ps}^\dagger a_{ps} + \tfrac{1}{2} V \times \sum_{\substack{p,p'=1,2,\ldots,N \\ s=+1,-1}} a_{ps}^\dagger a_{p's}^\dagger a_{p'-s} a_{p-s} \quad (\epsilon > 0), \tag{4.1}$$

which is commonly referred to as the Lipkin model. Energy levels of this system are easily obtained by introducing the quasispin operators

$$\begin{aligned} J_x &= \tfrac{1}{2} \sum_{p=1,\ldots,N} (a_{p+1}^\dagger a_{p-1} + a_{p-1}^\dagger a_{p+1}) , \\ J_y &= -\tfrac{1}{2} i \sum_{p=1,\ldots,N} (a_{p+1}^\dagger a_{p-1} - a_{p-1}^\dagger a_{p+1}) , \\ J_z &= \tfrac{1}{2} \sum_{\substack{p=1,\ldots,N \\ s=+1,-1}} s a_{ps}^\dagger a_{ps} , \end{aligned} \tag{4.2}$$

by which H can be rewritten as

$$H = \epsilon J_z + V(J_x^2 - J_y^2) . \tag{4.3}$$

The Hamiltonian commutes with

$$J^2 = J_x^2 + J_y^2 + J_z^2 , \tag{4.4a}$$

and the exact eigenstates may be classified in multiplets. In addition, H commutes with the operators

$$n_p = \sum_s a_{ps}^\dagger a_{ps} , \quad p = 1, \ldots, N , \quad p = 1, \ldots, N . \tag{4.4b}$$

Every n_p has eigenvalues 0, 1, or 2, as is seen from the relation $n_p^3 - 3n_p^2 + 2n_p = 0$. Since only single-particle states with unit eigenvalue of n_p are active, in the sense that they are affected by H, we will restrict our attention to states of the system for which all $n_p = 1$.

The eigenvalues of H always come in pairs of the opposite sign since H changes its sign under the rotation through 180° about the $x=y$ axis in the quasispin space.

The last useful symmetry of H is its commutativity with

$$\hat{\pi} = e^{i\pi J_z} . \tag{4.4c}$$

Following Ref. 14 we refer to $\hat{\pi}$ as the parity operator.

The quadratic dependence of H on J_x, J_y in the present model is the analog of the quadratic dependence on $\hat{\rho}$ in a general case. Application of the Hubbard-Stratonovich transformation linearizes the evolution operator of the model with respect to J_x and J_y,

$$e^{-iHT} = \int D\sigma \exp\left(iV \int_0^T (\sigma_x^2 - \sigma_y^2) dt\right) U_\sigma(T, O) , \tag{4.5}$$

$$U_\sigma(T, O) = \tau \exp\left\{-i \int_0^T dt \left[\epsilon J_z + 2V(\sigma_x J_x - \sigma_y J_y)\right]\right\} ,$$

where,

$$\sigma_x = \sigma_x(t) , \quad \sigma_y = \sigma_y(t) ,$$

and

$$D\sigma = D\sigma_x(t) D\sigma_y(t) .$$

Although the linearized Hamiltonian

$$h_\sigma = \epsilon J_z + 2V(\sigma_x J_x - \sigma_y J_y) \tag{4.6}$$

has the other symmetries of H, it does not conserve parity, since, unlike H (4.3), it is not invariant under rotation by 180° around the z axis for arbitrary $\sigma_x(t)$, $\sigma_y(t)$. Following the procedure of Sec. III, we evaluate the expression

$$\int_0^\infty dT e^{iET} \operatorname{tr} e^{-iHT} = \int_0^\infty dT\, e^{iET} \int D\sigma \exp\left(-V\int_0^T (\sigma_x^2 - \sigma_y^2) dt\right) \operatorname{tr} U_\sigma(T, O) \tag{4.7}$$

in the Hilbert space of N-fermion wave functions with $n_p = 1$ for $p = 1, \ldots, N$. We construct eigenvalues of U_σ using determinantal wave functions which, in general, are not eigenstates of J^2. Later we will show how an alternative basis built out of eigenstates of J^2 can be used as well.

We are thus looking for eigenstates of $U_\sigma(T, O)$ of the form

$$|\Psi\rangle = |a \prod_{p=1,\ldots,N} \phi_p\rangle . \tag{4.8}$$

Owing to the condition that $n_p = 1$, the single-particle wave functions may be written in the form

$$\phi_p = \begin{pmatrix} b_p \\ c_p e^{i\psi_p} \end{pmatrix} e^{-i\chi_p} , \tag{4.9}$$

with real b_p, c_p, ψ_p, and χ_p, and normalization $b_p^2 + c_p^2 = 1$. In (4.9) only the nonzero part of the $2N$ components is shown. The stationary-phase approximation performed on each term of the trace leads to the self-consistent field:

$$\begin{aligned} &\sigma_{x,y}^0(t) = \sum_{p=1}^N \sigma_{x,y}^{(p)}(t) , \\ &\sigma_x^{(p)}(t) = \langle \phi_p | J_x | \phi_p \rangle = b_p c_p \cos\psi_p , \\ &\sigma_y^{(p)}(t) = \langle \phi_p | J_y | \phi_p \rangle = b_p c_p \sin\psi_p . \end{aligned} \tag{4.10}$$

These equations have to be solved self-consistently along with the Schrödinger equations for the ϕ_p's of (4.9):

$$\left(i\frac{\partial}{\partial t} - h_{\sigma^0}\right) \phi_p = 0, \quad p = 1, \ldots, N \tag{4.11}$$

where h_σ is given by (4.6). The solutions should be periodic up to a phase $\phi_p(T) = e^{-i\alpha_p} \phi_p(0)$. From the parametrization (4.9) it follows that the latter condition is satisfied if

$$\begin{aligned} &\alpha_p = \chi_p(T) - \chi_p(0) , \quad b_p(T) = b_p(0) , \quad c_p(T) = c_p(0) , \\ &\text{and} \\ &\psi_p(T) = \psi_p(0) + 2\mu\pi \end{aligned} \tag{4.12}$$

for integer μ. One could in general allow for $b_p(T) = \pm b_p(0)$, $c_p(T) = \pm c_p(0)$ with appropriate changes in conditions for ψ_p and χ_p. However, as will be seen later, $b_p(t)$ and $c_p(t)$ cannot change their sign and therefore (4.12) is the only possible choice.

Energy levels are obtained from those solutions which satisfy the quantization condition

$$\sum_{p=1,\ldots,N} \left[i \int_0^T dt \phi_p^\dagger \frac{\partial}{\partial t} \phi_p - \alpha_p \right] = 2M\pi .$$

With the parametrization (4.9) this condition reads

$$\sum_{p=1}^N \int_0^T c_p^2 \dot{\psi}_p dt = 2M\pi . \tag{4.13}$$

In obtaining the last equation we used the normalization $b_p^2 + c_p^2 = 1$ together with (4.12). It is seen that the quantization condition (4.13) does not require the calculation of $\chi_p(t)$ and α_p. This is a consequence of the fact that in this special case, the only role of α_p is to specify the overall time-dependent phase factor χ_p in the single-particle wave functions.

In order to proceed with evaluation of (4.13) we first consider how this condition depends on N. For this purpose let us assume that one has found a self-consistent field σ^0. Each ϕ_p is an eigenstate of U_{σ^0}. For a given p only two orthogonal eigenstates exist, which we denote by

$$\phi = \begin{pmatrix} b \\ ce^{i\psi} \end{pmatrix}, \quad \phi' = \begin{pmatrix} b' \\ c' e^{i\psi'} \end{pmatrix} .$$

Every ϕ_p can thus be either ϕ or ϕ' and the many-body wave function (4.8) can symbolically be written as

$$\Psi = \phi^n \phi'^{N-n} , \tag{4.14}$$

where $0 < n < N$ and we have suppressed the dependence of the ϕ's on p, the antisymmetrization, and the overall time-dependent phase.

Since ϕ and ϕ' are orthogonal, it follows that

$$\begin{aligned} &bc = -b'c' , \\ &b^2 = c'^2 , \\ &c^2 = b'^2 , \\ &\psi = \psi' . \end{aligned}$$

The expressions for the self-consistent field σ^0, (4.10), and the quantization condition (4.13) are consequently simplified:

$$\sigma_x^0=[n-(N-n)]bc\cos\psi=(2n-N)bc\cos\psi,$$
$$\sigma_y^0=[n-(N-n)]bc\sin\psi=(2n-N)bc\sin\psi,$$
$$\sum_{p=1}^{N}\int_0^T c_p{}^2\dot{\psi}_p dt=n\int_0^T c^2\dot{\psi}\,dt+(N-n)\int_0^T b^2\dot{\psi}\,dt$$
$$=(2n-N)\int_0^T c^2\dot{\psi}\,dt+2\mu\pi=2M\pi. \tag{4.15}$$

Thus,

$$(2n-N)\int_0^T c^2\dot{\psi}\,dt=2m\pi \tag{4.16}$$

for integer m. In deriving Eq. (4.16) the normalization and the last relation of (4.12) were used.

It is seen that the dependence of σ_x^0, σ_y^0 and the quantization condition on N and n is only via the multiplicative factor $2n-N$. Therefore, without loss of generality we can study the case $n=N$ for which

$$\Psi=\phi^N. \tag{4.17}$$

Note that this function corresponds to a wave function in the ground-state ($J=N/2$) multiplet. Indeed, all the spinors ϕ_p of (4.9) are identical, i.e., "pointing to the same direction" in the quasispin space. The cases in which some of the spinors are "pointing in the opposite direction" ($n<N$) correspond to the other multiplets.

It is not difficult to find the dependence of c^2 on ψ in (4.16). For this purpose, still considering the case $n=N$, we define

$$\sigma_z^0=\langle\Psi|J_z|\Psi\rangle=\tfrac{1}{2}N(b^2-c^2)$$

and use the conservation of the Hartree energy

$$E=\epsilon\sigma_z^0+V(\sigma_x^{02}-\sigma_y^{02}). \tag{4.18}$$

For the case $n<N$, σ_z^0 dependence on N and n is similar to that of σ_x^0, σ_y^0. By substituting the expressions for σ_x^0, σ_y^0, and σ_z^0 in (4.18), one obtains after some algebra

$$c^2=c_\pm{}^2=\frac{1}{2}\left[1-\frac{\tilde{\epsilon}}{x}\pm\frac{1}{x}(\tilde{\epsilon}^2+x^2-4\tilde{E}x)^{1/2}\right], \tag{4.19}$$

where

$$\tilde{\epsilon}=\frac{\epsilon}{NV},\quad \tilde{E}=\frac{E}{N^2V} \tag{4.20}$$

and

$$x=\cos2\psi. \tag{4.21}$$

We have thus succeeded in expressing c^2 in terms of ψ and the energy. The quantization condition can now be rewritten in the simple form

$$N\int c^2 d\psi=2m\pi. \tag{4.22}$$

The integration boundaries will be discussed subsequently.

The problem of obtaining approximate energy levels of the system is thus reduced to finding solutions fo (4.22) with c^2 of (4.19) in the physical domain such that $0<c^2<1$ for $-1<x<1$.

One can already verify that the symmetry between states of energy E and $-E$ of the exact eigenvalues exists also for approximate energy levels. Indeed, if for a given value of E, c^2 satisfies (4.22), then

$$c^2(-\tilde{E},-x)=1-c^2(\tilde{E},x)$$

will also satisfy (4.22) and for every approximate level E, there is the corresponding level $-E$.

B. Approximate energy levels

The detailed analysis of the function (4.19) is performed in Appendix C and depends crucially on the position of the branch points of $c^2(x)$, i.e., the values of x for which

$$\tilde{\epsilon}^2+x^2-4Ex=0. \tag{4.23}$$

In this connection, two types of periodic c^2 orbits are found in Appendix C, for which $0<c^2<1$. The first corresponds to a change of ψ in the whole 2π interval with c^2 taking the values of the positive branch $c^2=c_+{}^2$. This is the case in which the two branch points are not real, or from (4.23)

$$|\tilde{E}|<\tilde{\epsilon}/2. \tag{4.24}$$

Figure 1 shows a periodic solution $c^2(\psi)$ of this type (denoted by the plus sign).

The second type of periodic, physical orbit is obtained when the branch points are both real and lie in the interval $x\in[0,1]$ or $x\in[-1,0]$. This happens if

$$\tfrac{1}{2}\tilde{\epsilon}<|\tilde{E}|<\tfrac{1}{4}(1+\tilde{\epsilon}^2), \tag{4.25}$$

and such a case is illustrated in Fig. 2. For $\tilde{E}>0$ ($\tilde{E}<0$) it consists of two closed orbits around $\psi=0$, π ($\psi=\frac{1}{2}\pi,\frac{1}{2}3\pi$) within the 2π interval $[-\frac{1}{2}\pi,\frac{1}{2}3\pi]$ ($[0,2\pi]$).

We shall refer to the two types of orbits shown in Figs. 1 and 2 as "spherical" and "deformed" orbits, respectively. The spherical and deformed ground states of Ref. 14 are special cases of these orbits as shown in Appendix C. There is no periodic orbit (with $0<c^2<1$) where the branch points are real and at least one of them lies out of the interval $x\in[-1,1]$. This implies that no solutions with

$$\tfrac{1}{4}(1+\tilde{\epsilon}^2)<|\tilde{E}|$$

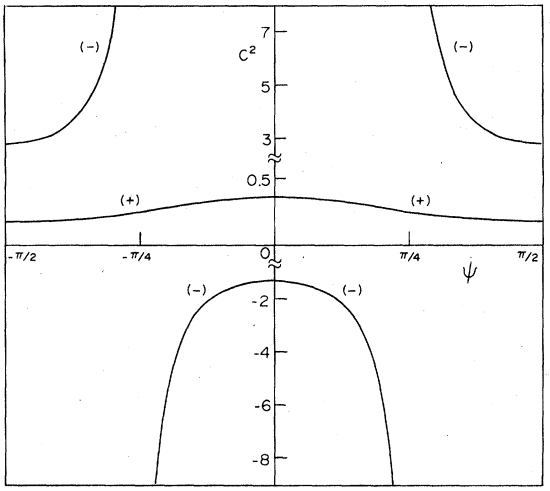

FIG. 1. The functions $c_+^2(\psi)$ and c_-^2 of Eq. (4.19) denoted by the plus and minus sign respectively, for parameters $\tilde{E} = 0.5$ and $\tilde{\epsilon} = 2.0$ in the spherical region. Only the c_+^2 branch is physical.

exist, as can be seen from (4.23). Furthermore, for the so-called weak-coupling case $\tilde{\epsilon} > 1$, deformed orbits do not exist as is clear from (4.25). In the strong-coupling case $\tilde{\epsilon} < 1$, both spherical and deformed orbits exist for $\tilde{E}$ satisfying (4.24) and (4.25), respectively.

With all the possible periodic orbits at hand we can now impose the quantization condition (4.22). For this purpose we define

$$I(\tilde{E}) = \int_{-\pi/2}^{\pi/2} c_+^2 d\psi \qquad (4.25a)$$

for the spherical case $|\tilde{E}| < \frac{1}{2}\tilde{\epsilon}$ and

$$I(\tilde{E}) = \oint c^2 d\psi \qquad (4.25b)$$

for the deformed orbit

$$\tfrac{1}{2}\tilde{\epsilon} < \tilde{E} < \tfrac{1}{4}(1+\tilde{\epsilon}^2).$$

The quantization condition then reads

$$I(E) = \frac{m\pi}{N}, \qquad (4.26)$$

where m is any integer for $|\tilde{E}| < \frac{1}{2}\tilde{\epsilon}$ and an even integer for

$$\tfrac{1}{2}\tilde{\epsilon} < \tilde{E} < \tfrac{1}{4}(1+\tilde{\epsilon}^2).$$

Slightly different definitions of $I(E)$ for

$$\tfrac{1}{4}(1+\epsilon^2) < \tilde{E} < \tfrac{1}{2}\tilde{\epsilon}$$

and the related conditions on m are discussed in Appendix C. Also discussed there is the dependence of I on $\tilde{E}$ in the weak- and strong-coupling regimes.

In Fig. 3, $I(\tilde{E})$ is plotted as a function of $\tilde{E}$ for four values of $\tilde{\epsilon}$. The first two $\tilde{\epsilon} = 2.0,\ 1.0$ belong to the weak-coupling category where only spherical orbits exist. The other two, $\tilde{\epsilon} = 0.5,\ 0.2$, are in the strong-coupling regime in which spherical and deformed orbits coexist. Points at which the $I(\tilde{E})$ plots cross the horizontal lines correspond to the $\tilde{E}$ values for which (4.26) is satisfied for an $N = 14$ particle system. Only positive energies are considered here, corresponding to $m < \frac{1}{2}N$. Odd- and even-m values are indicated by dashed and solid lines. Notice that $m = 1$ does not yield quantum states for $\tilde{\epsilon} = 0.5$ and $\tilde{\epsilon} = 0.2$ since (4.26) is not satisfied. Similarly, $m = 3$ yields no eigenstate for $\tilde{\epsilon} = 0.2$.

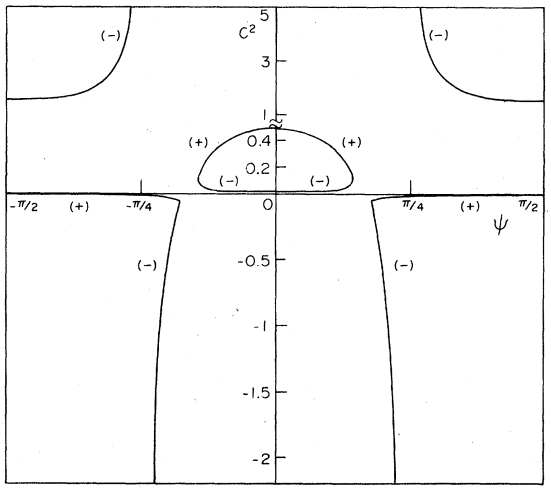

FIG. 2. Same as Fig. 1 for the parameters $\tilde{E} = 0.255$ and $\tilde{\epsilon} = 0.5$ in deformed region. Only the closed orbit is physical.

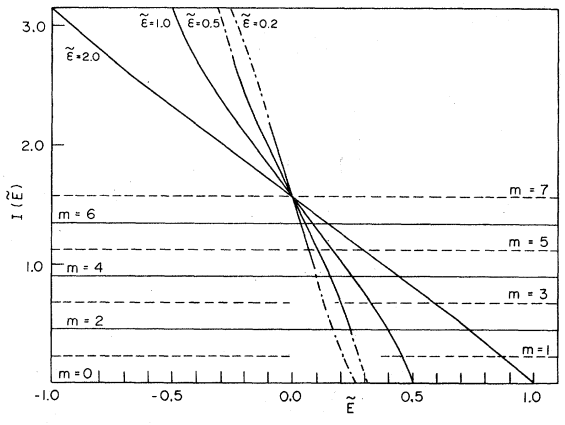

FIG. 3. The function $I(\tilde{E})$ of Eq. (4.25) for weak ($\tilde{\epsilon} = 2.0,\ 1.0$) and strong ($\tilde{\epsilon} = 0.5,\ 0.2$) couplings. Solid and dashed horizontal lines denote values of $m\pi/N$ for even and odd m, respectively, with $N = 14$. In deformed regions, denoted by dot-dashed lines, only even m yield energy levels.

From this figure and the analysis in Appendix C it is clear that in the weak-coupling case there are $N+1$ levels corresponding to $m=0,\ldots,N$. This is in correspondence with the exact number of levels of the ground-state multiplet. In the strong-coupling case, only either odd or even (cf. Appendix C) values of m should be used to define energy levels in the deformed region. However, these levels are double degenerate due to the existence of two closed orbits around $\psi=0$ and $\psi=\pi$.

In Fig. 4 we compare the approximate and the exact energy levels of a 14 particle system for a wide interval of $\tilde{\epsilon}$. Aside from the region $\tilde{E}=\tilde{\epsilon}/2$ discussed subsequently, overall agreement is seen to be very good. Odd-m and even-m levels [cf. (4.26)] are plotted with dashed and solid lines, respectively. The odd-m curves exist only for the spherical domain ($E/\epsilon<7$). The even-m levels in the deformed domain ($E/\epsilon>7$) are two-fold degenerate.

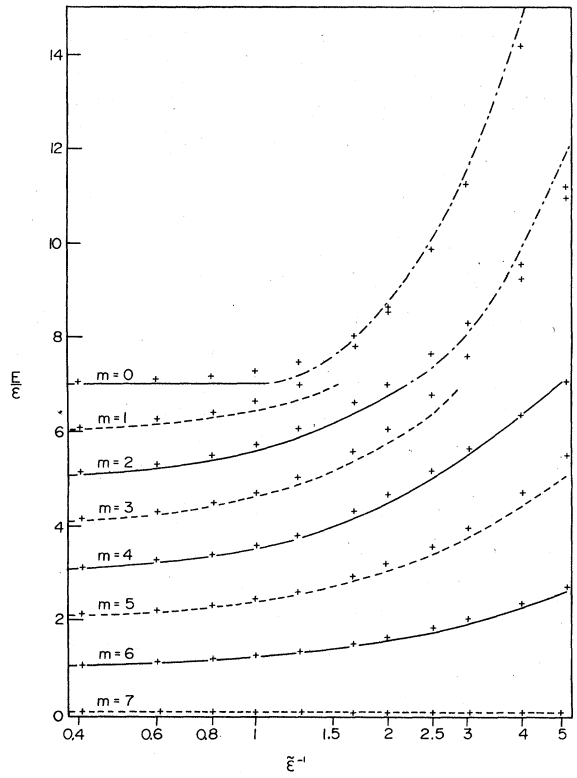

FIG. 4. Comparison of approximate and exact eigenvalues E/ϵ of a 14 particle Lipkin model for the ground-state multiplet as a function of $\tilde{\epsilon}^{-1}=NV/\epsilon$. Crosses denote exact eigenvalues, solid and dashed lines denote approximate levels for even and odd m, respectively, in the spherical region, and dot-dashed lines denote doubly degenerate deformed solutions. Because of symmetry, only non-negative levels are shown and $\tilde{\epsilon}^{-1}$ is logarithmically ruled for compactness.

C. Discussion of approximate solutions

Finally, we would like to discuss some qualitative aspects of the solutions just found, relating them to the exact solutions of the Lipkin model and to the SPA method for obtaining energy levels which was implemented here.

(*i*) *Existence.* In the general formulation of Secs. II and III above, no proof was given that periodic mean-field solutions of the self-consistent equations can be found. The present treatment of the Lipkin model system provides a specific case in which such solutions do exist. Thus, our nonlinear theory is in a position similar to the ordinary static HF, for which solutions can generally be found for cases of practical interest despite the lack of general existence theorems.

(*ii*) *Number of levels.* It was shown that the number of levels of the ground-state multiplet found by our calculation scheme is $N+1$ except for two possible extra levels in the strong-coupling regime in addition to the spurious unperturbed ground-state and highest excited state. Aside from these special cases discussed below, all the energy levels are obtained by this scheme.

(*iii*) *Types of solutions.* Due to the angular nature of the coordinate ψ, two types of periodic motion were found. Spherical solutions are those in which $c^2=c^2(\psi)$ varies along a single branch, c_+^2 and $\psi(T)=\psi(0)+2\pi$. The quasispin components (σ_x^p,σ_y^p), (4.10), are orbiting around (0, 0). The deformed solutions are those in which c^2 has branch points, and the periodic motion consists of progressing along one branch first, switching branches at the branch point, and going back along the other branch. The quasispin components (σ_x^p,σ_y^p) are now orbiting around the deformed configurations $[0,\pm c(1-c^2)^{1/2}]|_{x=1}$ at negative energies, and $[\pm c(1-c^2)^{1/2},0]|_{x=-1}$ at positive energies. The σ_z component in all cases is oscillating as well. Static solutions of the spherical and deformed domains are those for which the orbit shrinks to the single point at the center.

(*iv*) *Degeneracy.* The deformed solutions were found to be two-fold degenerate. This degeneracy is reflected in the two sign possibilities of the deformed configurations mentioned above. This degeneracy was noticed already by Agassi *et al.*[14] in the special case of the static, deformed Hartree-Fock ground state. Here excited states are also shown to have this property. The corresponding exact energy levels, shown in Fig. 4, are approximately degenerate. Their splitting decreases as the coupling increases.

(*v*) *Tunneling.* The removal of the degeneracy of the deformed static ground state was treated in Ref. 14 by the usual projection method. In our

approach it seems more appropriate to remove the degeneracy of both static and time-dependent states by taking into account the possibility of tunneling between closed orbits around $\psi=0$ and $\psi=\pi$ (or for $\tilde{E}<-\frac{1}{2}\tilde{\epsilon}:\psi=\pm\pi/2$).

(*vi*) *Symmetries*. The reason for the appearance of exact twofold degeneracy of the approximate solutions is that this solution breaks the exact parity symmetry of the Hamiltonian[14] as discussed previously in connection with Eq. (4.9).

(*vii*) *J quantum number*. Since h_σ commutes with J^2 for any $\sigma(t)$, the eigenstates of U_σ could have been chosen to have good J-quantum numbers. The ground-state multiplet wave function, Eq. (4.20), is an eigenstate of J^2 with eigenvalue $J=\frac{1}{2}N$, as may be verified by evaluating J^2 in a frame where $J_{z'}|\phi\rangle=\frac{1}{2}|\phi\rangle$. However, for $n\neq N$ in (4.14) Ψ is not an eigenstate of J^2. This is the result of using determinantal wave functions, and nondeterminantal wave functions which take the J^2 symmetry into account are discussed below.

(*viii*) n_p *symmetry and p independence*. All the functions Ψ of the form (4.8) are eigenfunctions of all of the occupation operators n_p (4.4). The p independence leads to a trivial degeneracy (by permutation of the p labels) of the energy levels, except for the case of the ground-state multiplet.

(*ix*) *Symmetry between states with energy E and* $-E$. This symmetry exists for both exact and approximate levels. It leads to the immediate conclusion that for even N systems there is a level with $E=0$ in each of its multiplets and the approximation is exact. For $n=\frac{1}{2}N$ $E=0$ is a static level, since $\sigma_x^0=\sigma_y^0=0$.

(*x*) *Comparison with RPA*. Ordinary and renormalized RPA calculations of ΔE, the excitation energy of the first excited state, were performed by Meshkov *et al.*[15] with the introduction of the model. Using their results for $N=14$, $\tilde{\epsilon}=1.25$ for calculating $(\Delta E)_{\text{approx}}/(\Delta E)_{\text{exact}}$ one finds 53%, 82%, and 89% for the ordinary linearization scheme and renormalized calculations to second and fourth order, respectively. The present calculation yields 94.8% for this ratio. As seen in Fig. 4, the spacing between the ground state and first excited state is actually less accurate than the level spacing near the center of the spectrum where the corresponding ratio is 98.6%. This is not surprising since the exact level at $E=0$ is obtained also by the approximation scheme. Aside from quantitative differences there are obvious qualitative differences between the current approximation and the RPA. For instance, the spacing between the excited states is expected to be equal in RPA, and there is no clear limit to the number of levels. The levels in the present study are not equally spaced, and their number is finite and except for pathological cases equal to the correct number of states in each multiplet.

(*xi*) *Breakdown of SPA*. It was shown in Appendix C that the unperturbed ground state is always a solution satisfying the quantization condition. In the weak-coupling regime, this is just the mean-field ground state. However, in the strong-coupling case this state is unstable and cannot be considered as a state in spite of the fact that the quantization condition is satisfied. The situation in this case is analogous to that of a particle in a symmetric double-well potential. The unperturbed ground state corresponds to the solution in which the particle stays on top of the barrier. Indeed, we saw that at $\tilde{E}=\pm\frac{1}{2}\tilde{\epsilon}$ many orbits are possible with smooth transition between them. In the analogous double well this motion corresponds to the oscillations of a particle at an energy equal to the height of the central barrier. Clearly, in this case the SPA is not applicable since the $\sigma(t)$ of the various possible solutions interfere. It is thus not surprising that in the region in which a level from the spherical domain crosses the top of the barrier into the deformed regime, the approximation is relatively poor and for even- (odd) m values an extra level appears for even- (odd) N systems.

(*xii*) *The multiplets*. By setting n of (4.14) to $0<n<N$, one obtains the rest of the multiplets by the same procedure, provided N is replaced by $2n-N$ in Eq. (4.17) and subsequent equations. These states are not eigenstates of J^2. Instead they are linear combinations of components belonging to all values of J satisfying $\frac{1}{2}|2n-N|<J<\frac{1}{2}N$.

(*xiii*) *Eigenstates of* J^2. It is easy to verify that any two spinors coupled to $j=0$ contribute nothing to the energy, σ^0, or S_{eff}. Therefore, if two particles are paired in this way and the rest have identical functions, the total J is that of the $N-2$ particles, namely, $J=\frac{1}{2}N-1$. The pairing of two such particles is done simply by taking the antisymmetric combination

$$|(\phi_{p+1}\phi_{p'-1})^{(0)}\rangle=(|\phi_{p+1}\phi_{p'-1}\rangle-|\phi_{p-1}\phi_{p'+1}\rangle)/\sqrt{2}.$$

Clearly, the lower J multiplets are obtained when more $j=0$ pairs are formed. This possibility emphasizes the fact that Slater determinants are not the only possible choice, and there are cases in which other wave functions are advantageous.

V. CONCLUSIONS

The quantum mean-field theory of bound states of finite nuclei presented in this work has several appealing features. Starting from an exact functional integral expression for the evolution opera-

tor, a periodic time-dependent Hartree-Fock mean field is seen to emerge naturally. There is no question as to whether or how to quantize as in many alternative formulations. No assumption of adiabaticity is involved and no explicit selection of a finite number of collective variables is required. The theory has been shown to have the proper static HF and small amplitude RPA limits, and yields an excellent approximation to the entire spectrum of the Lipkin model.

Several open questions arising during the course of this work merit comment. One difficulty concerns counting quantum states, and may be simply posed in the context of the RPA limit. It is known that some of the RPA states describe particle-hole excited states which can as well be associated with a static HF solution for a different set of occupation numbers $\{n\}$. Thus, different self-consistent solutions yield an approximation to the same state. Since substantial mathematical difficulties arise in attempting to add the contributions of distinct stationary solutions, cases of practical interest are presumably best resolved by selecting between alternative stationary solutions on physical grounds. In the case of the Lipkin model, except for pathological cases close to the boundary between spherical and deformed solutions, essentially all the states were accounted for correctly.

A second question arises concerning the relation between states having differing values of m in the quantization condition (3.28). In special cases the relation is unambiguous, such as RPA bands corresponding to different numbers of phonons in a particular mode, or the set of collective states of a multiplet with definite J in the Lipkin model. In the general case, although it is difficult to quantify the condition that two stationary quantized solutions are continuously related by smoothly increasing the period T and to resolve the 2π ambiguity in the quasienergies α_k/T, one nevertheless expects bands of nonlinear vibrational states to arise.

One of the most fundamental limitations of our entire formulation concerns our inability, in general, to assess the accuracy of the SPA. Although our procedure of selecting an observable, expressing it in terms of a functional integral, and applying the stationary-phase approximation appears quite general, there is no assurance that the SPA necessarily yields a meaningful approximation. For expectation values of few-body operators and modes in which many particles are participating in the same collective motion, one may plausibly expect the approximation to be viable. At the opposite extreme, the application of the method is questionable for expectation values of many-body operators or the overlap of arbitrary different N-body wave functions.

The formulation presented in this work has been deliberately restricted to evaluation of bound state energies. One might, however, consider evaluating the expectation value of any few-body operator Q by examining the residues of the quantity

$$\mathrm{tr}[Q(H-E)^{-1}]=\sum_{\nu}\frac{|\langle\psi_\nu|Q|\psi_\nu\rangle|^2}{E-E_\nu}, \tag{5.1}$$

which may be approximated by the method of Sec. III. For states corresponding to a static mean field, one can easily obtain the HF approximation to $\langle Q\rangle$. However, in the case of a time-dependent mean field, $\langle Q\rangle$ may acquire time dependence as a consequence of having broken the invariance with respect to time translation. To every broken symmetry, there corresponds a zero eigenvalue of the second variation matrix $\delta^2 S/\delta\sigma\delta\sigma$ necessitating a more careful treatment using the general methods of Ref. 9.

This brings us to the final open question which concerns the general problem of evaluating corrections to the SPA. The effective action, Eq. (3.12), in general depends on σ both through the evolution operator and through the states used to evaluate the trace. Instead of computing the full functional derivative with respect to σ of both the evolution operator and the basis, there are significant advantages of fixing the basis to be that which simply renders $\delta S=0$. First, since the use of the fixed basis breaks the symmetries of every term in $\mathrm{Tr}(H-E)^{-1}$ at the exact level, no zero eigenvalues will appear in the second variation of S in this fixed basis. Second, this fixed basis allows one to apply the method of Sec. II to evaluate the leading and higher quadratic corrections to SPA. The part of the discussion concerning the exchange and the self-energy terms in the mean field and the leading correction can be trivially repeated in the time-dependent basis of Sec. III. The similarity of this basis to the static HF basis will presumably enable evaluation of higher quadratic corrections as well, although we have not performed this calculation explicitly. Finally, the use of a fixed basis appears convenient also in a systematic treatment of the corrections higher than quadratic. Expanding $\mathrm{tr}\,U_\sigma$ in the formula

$$\mathrm{tr}U=\int D\sigma\exp\left(\tfrac{1}{2}i\int\sigma V\sigma\right)\mathrm{tr}U_\sigma$$

in powers of $\eta=\sigma-\sigma_0$, with σ_0 self-consistently defined by the basis in which the trace is evaluated, is a promising way to establish the connection of the present approach to perturbation theory. This seems to be especially useful in treating the problem of a hard core, which so far has been entirely ignored.

In addition to the preceding problems which merit further investigation, there exist a number of challenging prospects for future research. A number of formal connections with existing theory should be worked out. As mentioned in Sec. II, it should be straightforward to establish contact with the Hartree-Fock-Bogoliubov approximation. Projecting angular momentum by evaluating the integral

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{iM\phi}\,\mathrm{tr}\, e^{-i J_z \phi}(H-E)^{-1},$$

one may obtain the rotating frame approximation for deformed Hartree-Fock states and by further neglecting time derivatives obtain the adiabatic rotational limit.

Just as in the field theory case for which tunneling solutions may be obtained by continuing to imaginary time, so also the formalism in this present work may be extended to imaginary time to treat tunneling. One obvious application is an unambiguous quantum treatment of spontaneous fission. In addition, allowing tunneling solutions in the Lipkin model will split the twofold degeneracy in the deformed strong-coupling regime and allow a quantitative test of the approximation. Both applications will be addressed in subsequent publications.

Finally, the formalism presented in this work must ultimately be applied to real nuclei. As a first step, large amplitude vibrations and tunneling solutions are under investigation in a simple one-dimensional saturating model system. Generalizing from this system to three-dimensional calculations with realistic forces is only a matter of computer time, since existing TDHF technology may be applied directly. Thus, we believe this work provides a practical foundation for a quantitative theory of finite nuclei.

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APPENDIX A: DERIVATION OF THE QUADRATIC CORRECTION FACTOR

Application of the Gaussian integral

$$1=\frac{a}{\sqrt{\pi}}\int e^{-a^2 s^2} ds \tag{A1}$$

yields the identity

$$1=\int\cdots\int \prod_j \left(\frac{\lambda_j^{1/2}\Delta t\, ds_j}{\sqrt{2\pi i}} e^{i/2\ \Delta t^2 \lambda_j s_j^2}\right). \tag{A2}$$

Transformation to a general nondiagonal quadratic form using an arbitrary orthogonal matrix B

$$\begin{aligned} s_j &= \sum_k B_{jk}\Delta r \eta_k, \\ A_{jk} &\equiv \sum_i B_{ij} B_{ik}\lambda_i \end{aligned} \tag{A3}$$

yields the result

$$1=(\det A)^{1/2}\int\cdots\int \prod_j \left(\frac{\Delta t \Delta r}{\sqrt{2\pi i}} d\eta_j\right) \exp\left[\tfrac{1}{2} i \sum_{jk} A_{jk}(\Delta r \Delta t \eta_j)(\Delta r \Delta t \eta_k)\right]. \tag{A4}$$

Allowing j and k to denote space-time coordinates and taking the limit of infinitesimal Δr and Δt yields the appropriate measure for a general $A(x,t;x't')$ which is nonlocal in both space and time. We recover the measure appropriate to our functional integrals containing instantaneous potentials by writing

$$\int\int\int dx\, dx' dt \eta(xt) V(x-x')\eta(x't) \equiv \int\int\int dx\, dx' dt\, dt' \eta(xt)[V(x-x')\delta(t-t')]\eta(x't'), \tag{A5}$$

so that the measure in Eq. (2.6) is

$$D[\sigma(x,t)] = \lim \{\det[V(x-x')\delta(t-t')]\}^{1/2} \prod_j \left(\frac{\Delta t \Delta r}{(2\pi i)^{1/2}} d\sigma(x_j t_j)\right). \tag{A6}$$

Combining this equation with (A4), we obtain the desired result

$$\int D[\eta] \exp\left[\tfrac{1}{2} i \int A(xt, x't')\eta(xt)\eta(x't')\right] = \left\{\frac{\det[V(x-x')\delta(t-t')]}{\det A(xt;x't')}\right\}^{1/2}. \tag{A7}$$

APPENDIX B: EVALUATION OF $\partial S/\delta T$

To derive (3.21) we use the explicit expression (3.12) for S. The derivative of the first term is

$$\tfrac{1}{2}\int dx\,dx'\sigma(T)V\sigma(T)\,.$$

The derivative $d\alpha_j/dT$ appearing in the second term is evaluated as follows. We scale the time variable in Eq. (3.8) by defining

$$\eta=t/T \tag{B1}$$

and obtain

$$\left[-i\frac{\partial}{\partial\eta}+Th_{\sigma 0}(T\eta)\right]X(\eta)=\alpha X(\eta)\,, \tag{B2a}$$

$$X(1)=X(0)\,, \tag{B2b}$$

where

$$X(t/T)=u(t)\,. \tag{B3}$$

First-order perturbation theory then yields

$$\frac{d\alpha}{dT}=\frac{\int_0^1 d\eta\int dx X^*\frac{d}{dT}[Th_\sigma(T\eta)]X}{\int_0^1 d\eta\int dx\,X^*X}\,. \tag{B4}$$

Since

$$\frac{d}{dT}[Th_\sigma(T\eta)]=h_\sigma(t)+t(d/dt)h_\sigma(t)\,, \tag{B5}$$

one obtains, using the normalization (3.13),

$$\frac{d\alpha}{dT}=\frac{1}{T}\int dx\int_0^T dt\,u^*[h_\sigma(t)+t(d/dt)h_\sigma(t)]u\,. \tag{B6}$$

Partial integration of the second term gives

$$\int_0^T dtu^*(t)t(d/dt)h_\sigma(t)u(t)=Tu^*(T)h_\sigma(T)u(T)-\int_0^T dtu^*(t)h_\sigma(t)u(t)\,, \tag{B7}$$

where the terms containing time derivative of u^* and u cancel. Thus,

$$\frac{d\alpha_j}{dT}=\int dx\,u_j^*(T)h_\sigma(T)u_j(T)=\int dx\phi_j^*(T)h_\sigma(T)\phi_j(T) \tag{B8}$$

and

$$\frac{\partial S}{\partial T}=\tfrac{1}{2}\int dx\,dx'\sigma(T)V\sigma(T)-\sum_{j=1}^{\infty}n_j\langle\phi_j(T)|h_\sigma(T)|\phi_j(T)\rangle\,. \tag{B9}$$

When $\sigma=\sigma^0$ the right-hand side of this relation is $-E_{\mathrm{HF}}(T)$ and is independent of t.

APPENDIX C: PERIODIC ORBITS AND APPROXIMATE EIGENVALUES FOR THE LIPKIN MODEL

In the following analysis of the solution of Eq. (4.19) for periodic orbits and Eq. (4.22) for quantum levels, the weak-coupling case $\tilde{\epsilon}>1$ and the strong-coupling case $\tilde{\epsilon}<1$ are treated separately. The physical branches such that $0<c^2<1$ for $x\in[-1,1]$ can be obtained straightforwardly by setting algebraic inequalities of $c_\pm^2$. The following general observations simplify the analysis:

(i) Using the symmetry between states with energy E and $-E$, only $E>0$ values have to be considered, unless further insight is obtained by looking at $E<0$ too.

(ii) Both branches c_+^2 and c_-^2 are continuous functions of x and hence ψ except for c_-^2 which approaches $+\infty$ and $-\infty$ for negative and positive values of x, respectively, as x approaches zero.

(iii) It is easy to verify that

$$\begin{aligned} &c^2=0 \quad \text{if } \tilde{E}=\tfrac{1}{2}\tilde{\epsilon}\,,\\ &c^2=1 \quad \text{if } \tilde{E}=-\tfrac{1}{2}\tilde{\epsilon}\,, \end{aligned} \tag{C1}$$

independent of x. As a result, none of the branches can cross the $c^2=0$ and $c^2=1$ unless $\tilde{E}=\frac{1}{2}\tilde{\epsilon}$, $\tilde{E}=-\frac{1}{2}\tilde{\epsilon}$, respectively, provided the branches are not becoming complex in the region $-1<x<1$.

(iv) $c_\pm^2$ are complex in the interval (x_l,x_r), where the branch points x_l, x_r are the solutions of $\tilde{\epsilon}^2+x^2-4\tilde{E}x=0$, or specifically,

$$\begin{aligned} x_l&=2\tilde{E}-(4\tilde{E}^2-\tilde{\epsilon}^2)^{1/2}\\ x_r&=2\tilde{E}+(4\tilde{E}^2-\tilde{\epsilon}^2)^{1/2}. \end{aligned} \tag{C2}$$

Their real part $2\tilde{E}$ is positive ($\tilde{E}>0$).

1. Weak-coupling regime

In the weak-coupling regime $\tilde{\epsilon}>1$ the physical values of c^2 are obtained by noting that:

(a) None of the branches of c^2 are in the physical domain for $\tilde{E}>\frac{1}{2}\tilde{\epsilon}$.

(b) Only c_+^2 is physical for $0<\tilde{E}<\frac{1}{2}\tilde{\epsilon}$. Note (a) can be verified by observing that the branch points satisfy the inequalities $x_l>0$, $x_r>1$. In between these values $c_\pm^2$ is not real. For $x<x_l$,

$$\begin{aligned} &c_-^2(x)>1, \quad x<0,\\ &c_-^2<0, \quad 0<x<x_l \end{aligned}$$

as was pointed out by (ii) and (iii) above. Also, at the branch point x_l $c_+^2(x_l)=c_-^2(x_l)$. Hence c_+^2 is negative in the entire $[-1,x_l]$ interval, again by (ii) and (iii).

Note (b) follows from similar arguments except for the fact that x_l and x_r are now complex, and hence there are no branch points on the real x axis. c_-^2 is once again outside the interval $[0,1]$ by (ii) and (iii). c_+^2 is always between zero and

one since

$$0 < c_+^2(x=0) = \frac{1}{2} - \frac{\tilde{E}}{\tilde{\epsilon}} < \frac{1}{2}.$$

Note that for $\tilde{E} = \frac{1}{2}\tilde{\epsilon}$, c_+^2 is identically zero by (iii), and hence ψ, the relative phase of the upper and lower components of x, is irrelevant. This corresponds to a static Hartree solution.

The two branches c_+^2 and c_-^2 for $\tilde{\epsilon} = 2.0$, $\tilde{E} = 0.5$ are plotted as a function of ψ in Fig. 1, in the interval $[\frac{1}{2}\pi, \frac{1}{2}\pi]$. They are symmetric since $c_\pm^2$ depends on $x = \cos 2\psi$ only. c_+^2 (denoted by the plus sign) is confined to the interval $0 < c_+^2 < \frac{1}{2}$ and c_-^2 (denoted by the minus sign) is either larger than one or negative. c_-^2 diverges at $\psi = \frac{1}{4}x$. We conclude that all the possible solutions of the self-consistent problem in the weak-coupling regime are $c^2 = c_+^2$ for $-\frac{1}{2}\tilde{\epsilon} < \tilde{E} < \frac{1}{2}\tilde{\epsilon}$.

It remains now to check for which values of $\tilde{E}$ the quantization is met. It is convenient to define

$$I(\tilde{E}) = \int_{-\pi/2}^{\pi/2} c_+^2 d\psi . \tag{C3}$$

The quantization condition (4.22) then becomes

$$I(\tilde{E}) = (m/N)\pi . \tag{C4}$$

$I(\tilde{E})$ is a monotonically decreasing function of $\tilde{E}$ in the interval $\tilde{E}[-\frac{1}{2}\tilde{\epsilon}, \frac{1}{2}\tilde{\epsilon}]$, as can be verified by checking its derivative. Its values at $\tilde{E} = \pm\frac{1}{2}\tilde{\epsilon}$, are easily calculated. For $\tilde{E} = \frac{1}{2}\tilde{\epsilon}$, $c_+^2(\psi) = 0$ and $c_+^2(\psi) = 1$ for $\tilde{E} = -\frac{1}{2}\tilde{\epsilon}$. Hence,

$$I(\tfrac{1}{2}\tilde{\epsilon}) = 0, \quad I(-\tfrac{1}{2}\tilde{\epsilon}) = \pi .$$

One can easily verify that the symmetry between E and $-E$ implies in general

$$I(-\tilde{E}) = \pi - I(\tilde{E}). \tag{C5}$$

Accordingly,

$$I(\tilde{E} = 0) = \pi/2. \tag{C6}$$

The $\tilde{\epsilon} = 2.0$ and $\tilde{\epsilon} = 1$ curves of Fig. 2 show $I(\tilde{E})$ for these values of $\tilde{\epsilon}$, vs $\tilde{E}$. They cross each other at $E = 0$ owing to (C6), and they tend to be almost linear around this point, whereas they become slightly more curved around $\tilde{E} = \pm\frac{1}{2}\tilde{\epsilon}$. This curvature decreases as $\tilde{\epsilon}$ increases. All these features can be verified by checking the derivative of $I(\tilde{E})$.

For the quantization condition (C4), it is seen that there are $N+1$ values of m, $m = 0, 1, \ldots, N$, and $N+1$ corresponding values of $\tilde{E}$:

$$\tfrac{1}{2}\tilde{\epsilon} = \tilde{E}_0 > \tilde{E}_1 \cdots > \tilde{E}_N = -\tfrac{1}{2}\tilde{\epsilon} .$$

These values are indicated in Fig. 3, for the $N = 14$ fermion system, as the points at which $I(\tilde{E})$ for $\tilde{\epsilon} = 1.0$, 2.0 intersects the horizontal m lines. These solutions correspond to the spherical states discussed in Sec. IV.

2. Strong coupling regime

The study of the strong-coupling regime is simplified by distinguishing the three cases $|\tilde{E}| < \frac{1}{2}\tilde{\epsilon}$, $|\tilde{E}| = \frac{1}{2}\tilde{\epsilon}$ and $|\tilde{E}| > \frac{1}{2}\tilde{\epsilon}$. For $|\tilde{E}| < \frac{1}{2}\tilde{\epsilon}$ only c_+^2 is physical by the same arguments as in the weak-coupling regime. The only notable different is that in this spherical region the monotonically decreasing function $I(\tilde{E})$ never attains the values π and 0:

$$\pi > I(-\tfrac{1}{2}\tilde{\epsilon}) > I(\tfrac{1}{2}\tilde{\epsilon}) > 0 .$$

At $\tilde{E} = \frac{1}{2}\tilde{\epsilon}(\tilde{E} = -\frac{1}{2}\tilde{\epsilon})$ there are two physical solutions. The first is the static solution of the weak-coupling regime $c^2 = 0$ ($c^2 = 1$) and the second is the one obtained from the spherical solutions in the limit $\tilde{E} \to \frac{1}{2}\tilde{\epsilon}(-\frac{1}{2}\tilde{\epsilon})$. The two solutions coincide for $x < \tilde{\epsilon}(-\tilde{\epsilon} < x)$, allowing for an even more complicated periodic motion. As known already from the study of the weak-coupling case, the static solution satisfies the quantization condition. However, since there are two coalescing stationary-phase solutions, the applicability of SPA in its simplest form is questionable.

The interval $E > \frac{1}{2}\tilde{\epsilon}$ brings in a new type of solution, which exists only for

$$\tfrac{1}{4}(1+\tilde{\epsilon}^2) > |\tilde{E}| > \tfrac{1}{2}\tilde{\epsilon} . \tag{C7}$$

No "physical" solution exists for $\tilde{E} > (1+\tilde{\epsilon}^2)/4$, as can be proved by following the arguments used for $\tilde{E} > \frac{1}{2}\tilde{\epsilon}$ in the weak-coupling regime. Furthermore, since the branch points (C2) satisfy $0 < x_l < x_r < 1$, the same arguments will show that neither c_+^2 nor c_-^2 is in the physical interval $(0 < c^2 < 1)$ for $-1 < x < x_l$. At x_l they both coincide at a negative value. In the interval (x_l, x_r) $c_\pm^2$ are complex, but at x_r,

$$0 < c_+^2(x_r) = c_-^2(x_r) = \frac{1}{2}\left(1 - \frac{\tilde{\epsilon}}{x_r}\right) < \tfrac{1}{2} .$$

Thus, both c_+^2 and c_-^2 are physical in the interval $[x_r, 1]$, and the possible periodic motion consists of moving first along one branch and back along the other. Notice, however, that since $x = \cos 2\psi$, this motion can be localized around $\psi = 0$ or around $\psi = \pi$, leading to a two-fold degeneracy. The dependence of $c_\pm^2$ on ψ in the interval $-\pi/2 < \psi < \psi/2$ in the present case is illustrated in Fig. 2 for $\tilde{\epsilon} = 0.5$, $\tilde{E} = 0.255$. The solutions for $\frac{1}{4}(1+\tilde{\epsilon}^2) < \tilde{E} < \frac{1}{2}\tilde{\epsilon}$ are obtained once again by the symmetry between E and $-E$. We shall refer to all these solutions as deformed solutions. Notice that the static deformed ground state[14] (highest excited state) is obtained for

$$\tilde{E} = -\tfrac{1}{4}(1+\tilde{\epsilon}^2) \; [\tilde{E} = \tfrac{1}{4}(1+\tilde{\epsilon}^2)]$$

when the closed periodic motion shrinks into a point at $x = -1$ ($x = 1$).

For the deformed solutions, $I(\tilde{E})$ is defined as

$$I(E)=\int c^2 d\psi$$

$$=\int_{-\psi_r}^{\psi_r}(c_+^2-c_-^2)d\psi \quad (\tfrac{1}{4}1+\tilde{\epsilon}^2>\tilde{E}>\tfrac{1}{2}\epsilon), \quad \text{(C8a)}$$

$$I(\tilde{E})=\pi-\oint c^2 d\psi$$

$$=\pi\int_{-\psi_l}^{\psi_l}(c_+^2-c_-^2)d\psi\,[\tfrac{1}{4}(1+\tilde{\epsilon}^2)<\tilde{E}<-\tfrac{1}{2}\tilde{\epsilon}], \quad \text{(C8b)}$$

where

$$\psi_k=\cos^{-1}(x_k/2).$$

To within the additive constant π, $I(\tilde{E})$ is just the area enclosed by the closed orbit of Fig. 2. It is easy to verify that $I(\tilde{E})$ is once again a monotonically decreasing function and that

$$\lim_{E\to\pm\epsilon/2,0} I(\tilde{E})=\lim_{E\to\pm\epsilon/2,-0} I(\tilde{E}).$$

The constant π and the minus sign before the integral in the definition of $I(\tilde{E}<-\tilde{\epsilon}/2)$ are almost irrelevant for the quantization condition but do help to ensure continuity. Furthermore, $I(\tilde{E})$ goes once again from π to zero. The interval in the strong-coupling case is, however, $-[\frac{1}{4}(1+\tilde{\epsilon}^2), \frac{1}{4}(1+\tilde{\epsilon}^2)]$ rather than $[-\frac{1}{2}\tilde{\epsilon}, \frac{1}{2}\tilde{\epsilon}]$ of the weak-coupling case.

It remains now to check which self-consistent solutions satisfy the quantization condition (4.22). We recall that the condition applied to the weak-coupling case (C4) will result in $N+1$ distinct energy levels. However, now some of the levels, those of the deformed region, are two-fold degenerate. Two of these will always exist, the ground state and the highest excited state. A more careful application of (4.22) shows that the weak-coupling condition (C4) is applicable only in the spherical domain. In the deformed domain condition (4.22) is equivalent to

$$I(\tilde{E})=\begin{cases}\dfrac{2m+1}{N}\pi & \text{odd } N \text{ when } m>N/2\\ \dfrac{2m}{N}\pi & \text{otherwise.}\end{cases}$$

We can thus rewrite (4.22) for the strong-coupling regime as

$$I(\tilde{E})=\frac{m}{N}\pi\begin{cases}m \text{ integer for } -\frac{1}{2}\tilde{\epsilon}<\tilde{E}<\frac{1}{2}\tilde{\epsilon}\\ m \text{ even for } \frac{1}{2}\tilde{\epsilon}<\tilde{E}\\ m \text{ even for even } N,\ \tilde{E}<\frac{1}{2}\tilde{\epsilon}\\ m \text{ odd for odd } N,\ \tilde{E}<\frac{1}{2}\tilde{\epsilon}.\end{cases} \quad \text{(C9)}$$

In Fig. 3 the plots of $I(\tilde{E})$ vs $\tilde{E}$ in the strong-coupling regime are shown, corresponding to $\tilde{\epsilon}=0.5$ and $\tilde{\epsilon}=0.2$. The energy levels $\tilde{E}_m=E_m/N^2V$ are obtained from the points where these lines cross $m\pi/N$ lines indicated by horizontal lines. The lines of $m=1$ for the $\tilde{\epsilon}=0.5$ case and $m=1, 3$, for $\tilde{\epsilon}=0.2$ were excluded since they cross the $I(\tilde{E})$ plot in the deformed ($|\tilde{E}|>\frac{1}{2}\tilde{\epsilon}$) region where odd-$m$ values do not correspond to an energy level. On the other hand, energy levels obtained from the points in which $m=0$ and $m=0, 2, 4$, lines cross the $I(\tilde{E})$ curve of $\tilde{\epsilon}=0.5$ and $\tilde{\epsilon}=0.2$, respectively, yield twice degenerate levels.

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