Communications

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Constrained Hartree-Bogoliubov solutions as a basis for time-dependent calculations

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Starting from static constrained Hartree-Fock solutions, a numerically tractable method is proposed to study the inner excitation of a nucleus during collective deformations like fission. A prescription is proposed to determine the dynamics of one collective degree of freedom.

[NUCLEAR REACTIONS Fission from saddle to scission, time-dependent equations, constrained Hartree-Bogoliubov solutions as basis. Trajectory for collective variable from energy conservation.]

There has been considerable interest in time-dependent Hartree-Bogoliubov calculations as a method for studying collective dynamics. The wave function, at every point in time, is written in the form of a BCS ground state with the single-particle functions $\psi_n(\vec{r})$ and the pairing weights u_n and v_n determined "optimally."[1] A number of practical difficulties have been encountered with the implementation of the program, particularly with respect to the choice of initial conditions. We have no doubt that the problems are solvable. The purpose of this note, however, is to present an alternative approach, in the same spirit, which is numerically tractable and perhaps richer in content.

Static, constrained Hartree-Bogoliubov (CHB) solutions are now becoming available through the efforts of several groups.[2] These can be utilized as a representation for dynamic time-dependent calculations in a manner already demonstrated by the present authors in model calculations.[3] These calculations do not describe only adiabatic effects (as in time-dependent Hartree-Bogoliubov (HB) calculations), but also allow for nonadiabatic excitation (viscosity).

The formalism developed here is rather analogous to atomic collisions and molecular vibrations described in the adiabatic (Born-Oppenheimer) representation. Although we have set the discussion in the context of CHB, we could have chosen any appropriate constrained approximation as a basis, including exact solutions which have a certain deformation. For vibrational motion or fission dynamics, however, it is important to include pairing effects.

The starting point of constrained calculations is minimization of the expectation value of the many-body Hamiltonian H subject to the constraint that the expectation value of some operator, say Q, be fixed. We may regard Q as the quadrupole operator, but it may be more general than that. This is equivalent to minimizing the expectation value of

$$\mathcal{H} = H - \lambda Q, \tag{1}$$

where λ is a Lagrangian multiplier. Because of $d\langle H\rangle/d\langle Q\rangle = -\lambda$ this parameter vanishes at equilibrium[4] points (maxima and minima of the deformed ground state energy as function of $\langle Q\rangle$). In general $\langle H\rangle, \langle Q\rangle$, and other quantities are not single valued functions of λ. Therefore, we introduce another collective variable α, which could be $\langle Q\rangle$, and note that $\lambda(\alpha)$ is a single valued function. We take approximate solutions to

$$\mathcal{H}|n,\alpha\rangle = E_n(\alpha)|n,\alpha\rangle \tag{2}$$

as basis states. These functions form a complete orthonormal set for each $\alpha = \alpha(t)$.

We construct a time-dependent wave function

$$|\Psi(t)\rangle = \sum_n c_n(t)\exp\left\{-i\int^t \hat{E}_n[\alpha(t')]\,dt'\right\}|n,\alpha(t)\rangle \tag{3}$$

with $\hat{E}_n$ to be adjusted later. The $c_n(t)$ are determined by setting to zero the variation $\delta/\delta c_n(t)$ of the integral

$$I = \int dt\langle\Psi(t)|(H - i\partial/\partial t)|\Psi(t)\rangle. \tag{4}$$

This leads immediately to the coupled equations

$$i\dot{c}_n = \sum_{n'}\left(\langle n,\alpha|(H - i\dot{\alpha}\partial/\partial\alpha)|n',\alpha\rangle - \delta_{nn'}\hat{E}_n\right) \times c_{n'}\exp\left[i\int^t(\hat{E}_n - \hat{E}_{n'})dt'\right]. \tag{5}$$

We define

$$\hat{E}_n(\alpha) = \langle n,\alpha|H|n,\alpha\rangle = E_n + \lambda\langle n,\alpha|Q|n,\alpha\rangle.$$

Using (1), we find

$$i\dot{c}_n = \sum_{n'\neq n}\left\langle n,\alpha\left|\left(\mathcal{H} + \lambda Q - i\dot{\alpha}\frac{\partial}{\partial\alpha}\right)\right|n',\alpha\right\rangle \times c_{n'}\exp\left[i\int^t(\hat{E}_n - \hat{E}_{n'})dt'\right]. \tag{6}$$

Equation (6) is the exact Schrödinger equation if the basis set is complete. We now make two approximations in the context of the CHB procedure:
(1) We restrict consideration to the Hilbert space consisting of the (deformed) ground state of $\mathcal{H}$ and two quasiparticle ($2qp$) excitations. In the CHB basis, $\mathcal{H}$ has no matrix elements between the ground state and $2qp$ excitations.
(2) We ignore matrix elements $\langle 2qp'|\mathcal{H}|2qp\rangle$. In principle, these matrix elements exist, coming from the part of the Hamiltonian which contains four quasiparticle operators. This part is usually neglected in the HB procedure. In dropping these matrix elements, we still preserve the possibility of real quasiparticle excitations. (The more ambitious calculator may well find it feasible to keep these terms which, while generally cumbersome to store and handle, may still be tractable when a Skyrme force is used.)

We are now left with

$$i\dot{c}_n = \sum_{n'\neq n}\langle n,\alpha|(\lambda Q - i\dot{\alpha}\partial/\partial\alpha)|n',\alpha\rangle \times c_{n'}\exp\left[i\int^t(\hat{E}_n - \hat{E}_{n'})dt'\right]. \tag{7}$$

The matrix elements involve only single-particle operators. All that is needed to advance the equation in time are the functions of the static problem $\{\psi_n(\alpha), u_n(\alpha), v_n(\alpha)\}$, $\hat{E}_n(\alpha)$, $\lambda(\alpha)$, and initial conditions, and $\alpha(t)$. Here $\psi_n(\alpha)$ are single-particle wave functions. A method for advancing (7) in time is given in Ref. 3.

In order to determine $\alpha(t)$ we utilize conservation of energy for the Schrödinger equation

$$\frac{d}{dt}\langle H\rangle = 0, \tag{8}$$

where

$$\langle H\rangle = \mathcal{E}(t) = \sum_n |c_n|^2\hat{E}_n + \lambda\sum_{n\neq n'}\sum\langle n,\alpha|Q|n',\alpha\rangle \times\exp\left[i\int^t(\hat{E}_n - \hat{E}_{n'})dt'\right]. \tag{9}$$

Energy is not conserved automatically, since the restricted basis depends on time via the deformation. As proposed in Ref. 3, we can implement energy conservation numerically at each time step as follows: Consider that a solution is at hand to some time t, and one wishes to advance to time $t+\Delta t$. Try successively (say) two values of $\dot{\alpha}$, namely $\dot{\alpha}_1$ and $\dot{\alpha}_2$ which are assumed appropriate to the midpoint $t+\frac{1}{2}\Delta t$ for advancing Eq. (7) [$\alpha(t+\frac{1}{2}\Delta t)$ is also required]. These will lead, respectively, to two values $\mathcal{E}_1(t+\Delta t)$ and $\mathcal{E}_2(t+\Delta t)$ of the energy. Linear interpolation yields

$$\dot{\alpha}(t+\tfrac{1}{2}\Delta t) = \frac{1}{\mathcal{E}_2 - \mathcal{E}_1}[(\langle H\rangle - \mathcal{E}_1)\dot{\alpha}_2 + (\mathcal{E}_2 - \langle H\rangle)\dot{\alpha}_1]. \tag{10}$$

This can be iterated if higher accuracy is required.

In Ref. 3, where this method was proposed, we used a classical residual, collective mass term $\frac{1}{2}B_0\dot{\alpha}^2$ for the protons for the determination of $\dot{\alpha}(t+\frac{1}{2}\Delta t)$.

It is necessary to assume some initial set of amplitudes $c_n(0)$. The initial $\dot{\alpha}(0)$ is not important, since $\dot{\alpha}$ will be determined at the next half step by energy conservation. However, the $c_n(0)$ can reasonably be assumed to be the first order time-dependent perturbation expression by assuming some $\dot{\alpha}(0)$:

$$c_n(0) = -i\dot{\alpha}(0)\frac{\langle n,\alpha|\partial/\partial_\alpha|0,\alpha\rangle}{E_n - E_0}, \quad n\neq 0$$
$$c_0(0) = \left(1 - \sum_n{}'|c_n(0)|^2\right)^{1/2}, \tag{11}$$

where we have assumed starting at an equilibrium point $\lambda = 0$. Conditions (11) represent, in first order, minimum excitation energy conditions for a given $\dot{\alpha}$. The energy constant for all times is determined by the $c_n(0)$. The new $\dot{\alpha}(\frac{1}{2}\Delta t)$ may be somewhat different from the assumed $\dot{\alpha}(0)$ because of failure of first-order perturbation theory, but henceforth $\dot{\alpha}(t)$ should be a smooth function of time.

The use of a CHB basis set permits the calculation of classical dynamics along a one-dimensional trajectory in a manner which is numerically tractable. The method should be of special interest in the problem of fission, since it not only yields (implicitly) the inertia but also intrinsic excitation (viscosity).

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[1]D. J. Rowe, in *Fundamentals in Nuclear Theory, Trieste 1967* (IAEA, Vienna, 1967), p. 531.

[2]M. Brack and P. Quentin, in *Proceedings of the Third International Atomic Energy Agency Symposium on the Physics and Chemistry of Fission, Rochester, 1973* (IAEA, Vienna, 1974), p. 231; W. H. Bassichis and D. Tuerpe, Phys. Rev. C 8, 1146 (1973).

[3]G. Schütte and L. Wilets, in *Proceedings of the Third International Atomic Energy Agency Symposium on the Physics and Chemistry of Fission, Rochester, 1973* (see Ref. 2), p. 503; and Nucl. Phys. (to be published).

[4]W. H. Bassichis, A. K. Kerman, C. F. Tsang, D. G. Tuerpe, and L. Wilets, in *Magic Without Magic: John Archibald Wheeler, a Collection of Essays in Honor of His 60th Birthday*, edited by J. R. Klauder (Freeman, San Francisco, 1972).