QUANTUM MEAN-FIELD THEORY OF COLLECTIVE

DYNAMICS AND TUNNELING

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*This work is supported in part through funds provided by the U.S. DEPARTMENT OF ENERGY (DOE) under contract DE-AC02-76ER03069

To be published in the Proceedings of the Second International Conference on Recent Progress in Many-Body Theories, Mexico City, Jan. 12-16, 1981.

CTP #909
January 1981

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Introduction

A fundamental problem in quantum many-body theory is formulation of a microscopic theory of collective motion. For self-bound, saturating systems like finite nuclei described in the context of non-relativistic quantum mechanics with static interactions, the essential problem is how to formulate a systematic quantal theory in which the relevant collective variables and their dynamics arise directly and naturally from the Hamiltonian and the system under consideration. In collaboration with Shimon Levit and Zvi Paltiel, significant progress has been made recently in formulating the quantum many-body problem in terms of an expansion about solutions to time-dependent mean-field equations. The technical details of this approach are presented in detail in Refs. 1-3, and only the essential ideas, principal results, and illustrative examples will be summarized here.

The mean-field is an obvious candidate to communicate collective information. Possessing the infinite number of degrees of freedom of the one-body density matrix, it has access to all the shape and deformation degrees of freedom one intuitively believes to be relevant to nuclear dynamics. The static mean-field theory with appropriate effective interactions, commonly referred to as the Hartree Fock approximation, quantitatively reproduces the radial distributions and shapes of spherical and deformed nuclei throughout the periodic table. The time-dependent Hartree Fock (TDHF) approximation and its RPA limit for infinitesimal fluctuations similarly yields a reasonable description of transition densities to excited states, fusion cross sections in heavy ion reactions, and strongly damped collisions.

Whereas the mean field is thus a compelling foundation for a microscopic theory of collective motion, the TDHF initial value problem is an inappropriate starting point for a systematic quantum theory. Stimulated by developments in quantum field theory in which systematic expansions are developed about the solution to the corresponding classical field equations, we have developed a conceptually unambiguous quantum theory of collective motion. An exact expression for an observable of interest is written using a functional integral representation for the evolution operator, tractable time-dependent mean field equations are obtained by application of the stationary-phase approximation (SPA) to the functional integral, and corrections to the lowest-order theory may be systematically enumerated.

Outline of Approach

The essential steps in the method are as follows. First, one selects a few-body operator corresponding to a physical observable of interest and then one expresses its expectation value in terms of the evolution operator. For example, to calculate the bound state spectrum and the expectation value of any few-body operator $\mathcal{O}$ in any bound state, one may evaluate the poles and residues of the following expression:

$$-i\int dT e^{iET}\mathrm{tr}\,\mathcal{O}e^{-iHT} = \sum_n \frac{\langle n|\mathcal{O}|n\rangle}{E-E_n+i\epsilon} . \tag{1}$$

Next, one utilizes an appropriate functional integral representation for the many-body evolution operator. One particularly simple choice is the Hubbard-Stratonovich transformation used in Ref. 5

$$Te^{-\frac{i}{2}[\hat\rho v\hat\rho]} = \int D[\sigma]e^{\frac{i}{2}[\sigma v\sigma]}\,Te^{-i[\sigma v\hat\rho]} , \tag{2}$$

where the brackets denote the following integral

$$[\sigma v\rho] \equiv \int dx_1 dx_2 dx_3 dx_4 dt\,\sigma(x_1,x_2;t)\,v(x_1x_2x_3x_4)\,\rho(x_3,x_4;t) , \tag{3}$$

$\hat\rho$ is the interaction representation operator

$$\hat\rho(x,x';t) \equiv e^{iH_0t}\psi^+(x)\psi(x')e^{-iH_0t} , \tag{4}$$

and T denotes a time ordered product. The evolution operator corresponding to a Hamiltonian containing two-body interactions is thus replaced by an integral over an infinite set of evolution operators containing only one-body operators. A second alternative is to break the evolution into very small time steps between each of which an overcomplete set of Slater determinants is inserted[6,7]

$$\langle\psi_f|e^{-iHT}|\psi_i\rangle = \langle\psi_f|\ldots e^{-iH\Delta T}\int du(z)|\psi(z)\rangle\langle\psi(z)|e^{-iH\Delta T}\ldots|\psi_i\rangle . \tag{5}$$

The theory is rendered manageable by virtue of a simple choice of the measure $du(z)$ which efficiently handles the overcompleteness. A third alternative is to use Grassman variables as in field theory,[8] so that the trace of the exponential of the action becomes[9]

$$\mathrm{tr}\,e^{iS} = \int D[Z^*,Z]e^{i\int\left[Z^*\left(i\frac{\partial}{\partial t}-T\right)Z-\frac{1}{2}Z^*Z^*vZZ\right]} . \tag{6}$$

Finally, for any of these functional integral representations when suitably generalized to include exchange, application of the SPA yields TDHF equations plus a systematic hierarchy of corrections.

The essence of the program is exemplified by applying it to the trivial problem of one-dimensional quantum mechanics in the potential shown in Fig. 1, for which case we may write

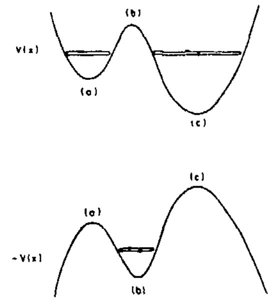

Fig. 1 Sketch of a double well with two classically allowed regions separated by one classically forbidden region.

$$\mathrm{Tr}\frac{1}{H-E} = i\int dTe^{iET}\int dq\langle q|e^{-iHT}|q\rangle$$

$$= i\int dTe^{-ET}\int dq\int D[q(t)]e^{iS[q(t)]}\Big|_{q(t)=q(0)=q} , \tag{7}$$

where $S[q(t)]$ in the Feynman path integral denotes the classical action. Application of the SPA to $\int D[q(t)]$ requires that $q(t)$ must satisfy the classical equation of motion

$$m\frac{d^2}{dt^2}q = -\nabla V \tag{8}$$

and application of the SPA to $\int dq$ requires that the momentum at time T equal that at time 0. Thus, we obtain

$$\mathrm{Tr}\frac{1}{H-E} = i\int_0^\infty dt\sum_{q_{cl}} e^{i(ET+S(T))} \equiv i\int dT\sum_{q_{cl}} e^{iW(T)} , \tag{9}$$

where $S(T)$ is the action for a periodic solution to the classical equation of motion and the sum $\sum_{q_{cl}}$ includes all such periodic classical solutions.

Finally, the SPA is applied to the time integral in Eq. (9), giving rise to both real and complex stationary values of the period. Real periods simply correspond to multiples of the fundamental periods for classical oscillations around minima (a) and (c) in Fig. 1 such that the classical energy equals E. The period and contribution to the reduced action $W(T)$ of Eq. (9) for periodic solutions in region a (and similarly for region c) are

$$T_a = 2\int dq\sqrt{\frac{m}{2(E-V(q))}} , \tag{10}$$

and

$$W_a = \oint p\dot q\,dt = 2\int\sqrt{2m(E-V(q))}\,dq . \tag{11}$$

The meaning of classical solutions for imaginary time is most evident if one simply replaces (it) by in the equations of motion. The two resulting factors of in Eq. (8) are then equivalent to reversing the sign of . As sketched in Fig. 1, this has the effect of interchanging classically allowed and forbidden regions, so one now has periodic solutions in region b with imaginary period and reduced action

$$iT_b = \bar{T}_b = 2\int dq \Big/ \sqrt{2(V(q)-E)} \quad , \tag{12}$$

and

$$iW_b(E) = \bar{W}_b(E) = 2\int \sqrt{2m(V(q)-E)}\,dq \quad , \tag{13}$$

Combining all integral numbers of periods in the three regions thus yields an infinite sequence of stationary points $T_{\ell mn} = \ell T_a + mT_c - in\bar{T}_b$ and the corresponding sum over classical periodic trajectories in Eq. (18) yields multiple geometric series which sum to

$$Tr\frac{1}{H-E} = \frac{e^{iW_a}+e^{-\bar{W}_b}+e^{iW_c}-2e^{i(W_a+W_c)}}{\left(1-e^{iW_a}\right)\left(1-e^{iW_c}\right)-e^{-\bar{W}_b}} \quad . \tag{14}$$

For the case of a single well, in which case regions (b) and (c) don't exist, this yields poles at energies E_n such that

$$W_i(E_n) = \int pdq = 2n\pi \quad . \tag{15}$$

Eq. (15) differs from the usual Bohr-Sommerfeld quantization condition (2n+1) only because we have neglected phase factors arising from quadratic corrections to the SPA. In the case of spontaneous decay of a quasi-stationary state, region (c) is elongated to extend throughout an arbitrarily large normalization box, and one observes that W_c then yields a vanishing contribution to the smoothed level density

$$\rho_\gamma \equiv \frac{1}{\pi}\, Im Tr\frac{1}{H-E+i\gamma} \approx \left[\left(\frac{e^{-\bar{W}_b}}{2}\right) + \sin\frac{W_a}{2}\right] \tag{16}$$

The level density, Eq. (16), exhibits quasi-stationary states with energies given by Eq. (15) and widths

$$\Gamma_n = 2\left(\frac{\partial W_a}{\partial E}\right)e^{-\bar{W}_b(E_n)} = T_a e^{-\bar{W}_b(E_n)} \tag{17}$$

which agree with the familiar WKB result to within a factor 1/2 discussed in Ref. 10.

Application to Many-Body Problem

Straightforward application of the same program to the many-body problem results in application of the SPA to the T and integrals in an expression of the form

$$\int dTe^{iET}tre^{-iHT} \cdot \int dTe^{iET} D[\psi]e^{iS[\psi]} \quad , \tag{18}$$

where

$$\ldots \; tr \ln \ldots \quad ,$$

and yields three distinct classes of solutions.

Time-independent solutions to the SPA equations reproduce familiar HF theory. The quadratic corrections to SPA produce the RPA ground state correlations, and the systematic evaluation of higher corrections generates standard perturbation theory. Aside from providing a terse and elegant derivation of perturbation theory, this functional integral approach has the additional advantage of dealing efficiently with constraints, such as those arising in gauge theories.

A second class comprises time-dependent solutions with real period which correspond to eigenfunctions of large-amplitude collective motion. A set of N single-particle wave functions obey the following eigenvalue equation

$$\left[-i\frac{\partial}{\partial t}+K+tr\,v\rho\right]\phi_i(x,t) = \epsilon_i\phi_i(x,t) \tag{19}$$

subject to the periodic boundary condition

$$\phi_i\left(x,\frac{T}{2}\right) = \phi_i\left(x,-\frac{T}{2}\right) \quad , \tag{20}$$

where the self-consistent mean field satisfies

$$\rho(x,x',t) = \sum_i \phi_i^*(x',t)\phi_i(x,t) \quad , \tag{21}$$

K denotes the kinetic energy operator and the allowed values of the period are specified by the quantization condition

$$\int dx \int_{-T/2}^{T/2} dt\,\phi^*(x,t)\,i\frac{\partial}{\partial t}\phi(x,t) = n2\pi \quad . \tag{22}$$

Clearly the non-linear differential Eqs. (19-21) in four space-time dimensions have the same general structure as the static Hartree equations in three space dimensions, and they may be solved by the usual iterative procedure. Application of this method to the ground state multiplet of the spectrum of the Lipkin model yields the results shown in Fig. 2. Further discussion of large amplitude collective motion using this general approach may be found in Ref. 1.

The third class of solutions is made up of time-dependent solutions with imaginary period corresponding to tunneling phenomena in classically forbidden domains. In this case, the single-particle Equations (19) are replaced by

$$\left[\frac{\partial}{\partial\tau}+K+tr\,v\rho\right]\phi_i(x,\tau) = \epsilon_i\phi_i(x,\tau) \quad , \tag{23}$$

with the same periodic boundary condition (20) and the self-consistent mean field

$$\rho(x,x',\tau) = \sum_i \phi_i(x',-\tau)\phi_i(x,\tau) \quad . \tag{24}$$

Of particular physical interest are solutions which in the limit as $T/2 \to \infty$ approach the HF stationary local minimum for a fissioning nucleus and evolve near T 0 toward the entrance to the classically allowed domain near the scission point for two fission fragments. Such solutions will be denoted "bounces", following Coleman, and bear great formal similarity to the "pseudoparticles and "instantons" [illegible] investigated extensively in field theory. Whereas the Euclidean solutions arising in field theory have trivial spatial dependence, being either constant or spherically symmetric in space-time, the non-trivial spatial dependence of the present "bounce" solutions is crucial to the physics and precludes analytic solution even for schematic models. Furthermore, for a nucleus possessing many decay channels such as symmetric fission, asymmetric fission, alpha, proton, or neutron decay, there will exist several distinct well-separated bounces, and the analog of the width in Eq. (17) is the sum of partial widths:

$$\Gamma = \sum_m \Gamma^{(m)} , \qquad (25)$$

where each partial width is calculated from the action determined for the bounce solution for the appropriate channel

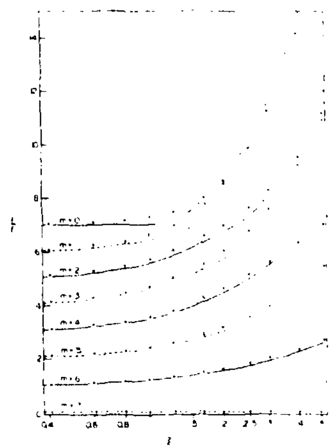

Fig. 2 Exact Lipkin spectrum (crosses) compared with the mean-field approximation as a function of $\chi=NV/\epsilon$. The particle number N in this case is 14, V is the strength of the interaction coupling pairs of particles in the two levels, and ϵ is the energy separation of the two levels. The dot-dash curves denote doubly degenerate approximate solutions and the other curves are non-degenerate.

$$\Gamma^{(m)} = 2T_m e^{-\int_{-T/2}^{T/2} d\tau\, \psi(x,\tau)\frac{\partial}{\partial\tau}\psi(x,\tau)} \qquad (26)$$

To make these bounce solutions more concrete, it is useful to consider a saturating model system of nuclei in one spatial dimension interacting with an effective interaction of the Skyrme form. The analog of the Coulomb force is adjusted such that a 16-particle system is unstable with respect to fission into two 8-particle daughters which are in turn stable with respect to further decay into 4-particle granddaughters. The constrained HF energy as a function of $\langle x^2\rangle$ for the 16-particle system is shown in Fig. 3, and displays the expected form of a fission barrier. The self-consistent single-particle solutions to Eqs. (23), assuming spin-isospin degeneracy 4, are shown in Fig. 4 at the two turning points, $\tau=-T/2$ and $\tau=0$. As expected, the determinant of these wave functions corresponds to the 16-particle [illegible] at $\tau=-T/2$ and closely approximates the product of two [illegible] nearly-separated fragments at $\tau=0$. The corresponding densities [illegible] Fig. 5 for successive times between $\tau=-T/2$ and $\tau=0$.

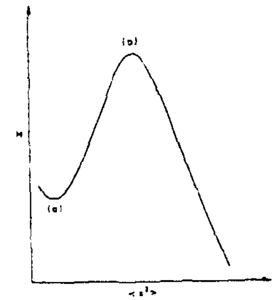

Fig. 3 The constrained energy of a 16-particle model system as a function of $\langle x^2\rangle$.

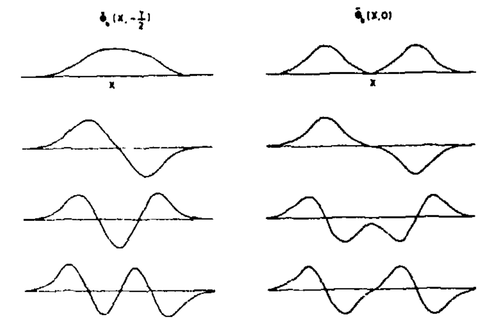

Fig. 4 Self consistent single-particle wave functions as a function of x at times $\tau=-T/2$ and $\tau=0$ for the bounce solution for spontaneous fission of a 16-particle model system.

Solution of Eqs. (22) in four space-time dimensions is obviously computationally more cumbersome, but has been accomplished for a range of nuclei up to A=32. In these calculations, the proton charge has been increased to obtain appropriate values of the fissility, and preliminary results for the fission of ^{8}Be are shown in Fig. 6. Although spurious cm motion problems prevent quantitative comparison of this particular calculation with experiment, this result does demonstrate the feasibility of obtaining bounce solutions with the appropriate properties and shows that all the relevant shape degrees of freedom are incorporated in this self-consistent theory.

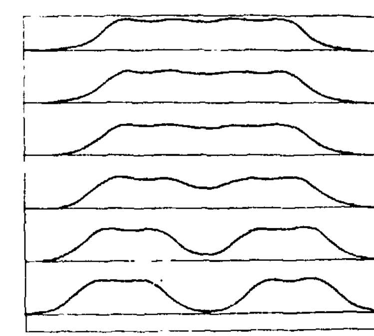

Fig. 5 The density $\rho(x,\tau)$ for the same system as in Fig. 4 as a function of x at successive times from $\tau=-T/2$ to $\tau=0$.

Outlook

Clearly, many other applications of quantum mean-field approximations arising from [illegible] functional integral expressions are possible. One should eventually be [illegible] quantitatively understand the systematics of fission lifetimes in heavy nuclei, including shell effe[illegible] and the competition between symmetr[illegible] and a[illegible]metric decay channels. Similarl[illegible], excited states of soft transitional nuclei involving very large amplitude collective vibrations should be well described by the present theory. Reaction theory poses many important and challenging problems. Although it is possible to write exact functional integral expressions for S-matrix elements,[illegible] the key to a meaningful reaction theory is finding an appropriate functional integral expression for relevant expectation values of few-body operators, such as mean fragment charge, mass, or excitation energy, which yields numerically tractable mean-field equations. In contrast to the TDHF initial value problem, which describes the most probable outcome, such functional integral expressions for specific observables can address specific components of interest, even those which are exponentially small relative to the most probable component. This, then, is a natural language to address such diverse and important questions as superheavy nucleus formation in heavy ion collisions, and tunneling phenomena in light-ion collisions associated with quasi-molecular states and the resonance behavior in such systems as [illegible]Mg. Generalization to finite temperature is straightforward and offers an ideal framework from which to consider the equation of state of hot matter at subnuclear density in neutron stars, as well as a variety of other finite temperature many-body systems.

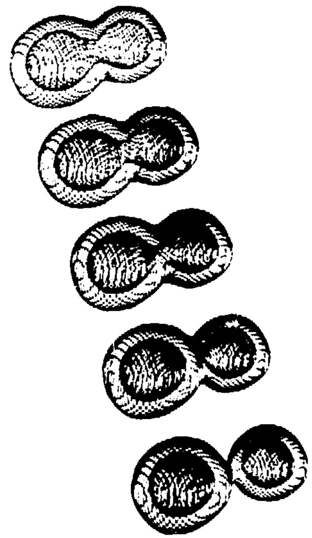

Fig. 6 Three dimensional perspective plots of surfaces of constant density for fission of [illegible]Be. The inner and outer surfaces correspond to densities of 1/3 and 2/3 nuclear matter density respectively and the sequence of shapes run from [illegible]=-T/2 to [illegible]=0.

In summary, the quantum mean-field theory presented here offers promise in a variety of applications in non-relativistic many-body theory. The principal unresolved challenges at present are understanding the validity and accuracy of the [illegible] and developing more powerful approximation techniques to deal with the resulting time-dependent mean field equations.

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