# **Nuclear mean-field theory**

This theory provides insight into diverse nuclear phenomena ranging from ground-state properties of nuclei and the matter in neutron stars to the dynamics of heavy-ion collisions and spontaneous fission.

John W. Negele

One of the fundamental challenges common to all areas of physics is to understand the properties of systems having large or infinite numbers of degrees of freedom in terms of known underlying interactions. Simply knowing the Schrödinger equation and Coulomb's law, for example, is not sufficient to let us understand the chain through which atoms form molecules, which, in turn, beget macromolcules, which eventually aggregate into a biological object with a life of its own. Nor has knowledge of the Lagrangian for quantum chromodynamics yet yielded an understanding of hadrons. The physics of systems with many degrees of freedom often differs in crucial ways from what we understand for simple systems.

Among these complex many-body problems, the ground-state structure and low-energy dynamics of atomic nuclei pose a unique challenge: to understand the physics of small drops of a dense, strongly interacting quantum liquid. The underlying interactions are sufficiently well known that the essential questions are those of many-body physics: the nature of the ground state of bulk matter, the shape and radial distribution of the nuclear surface, the interplay between singleparticle and collective degrees of freedom, and the nature of the fundamental excitations.

These questions are similar to those posed for aggregates of weakly interacting particles-such as electrons orbiting an atom or moving through a

crystal. In those cases it is often useful

to assume that the dominant effect of all the other particles on a single particle is to provide a smooth field in which the particle moves. At first sight, it is astonishing that a theory even remotely resembling this meanfield approximation familiar to us from atomic physics should have anything to do with dense, strongly interacting systems such as nuclei. In recent years, however, nuclear mean-field theory has begun to yield a quantitative description of nuclear structure and

There is, furthermore, a wealth of experimental information with which to test our theoretical understanding of nuclear structure and dynamics. In contrast to other dense quantum liquids, such as liquid helium, which thus far may only be studied in bulk, finite nuclei are accessible to diverse and precise probes. Nuclear charge, current and magnetization densities have been measured in detail with electromagnetic probes; excited states with virtually any desired quantum numbers have been explored with hadronic probes; and large-amplitude collective motions have been studied in processes ranging from spontaneous and induced fission to collisions between heavy nuclei.

These experimental and theoretical developments1 are providing more and more support for a static nuclear meanfield theory and for its time-dependent and finite-temperature generalizations. Figure 1 shows an example of one of the phenomena-spontaneous fission-that one can now calculate using the mean-field theory.

#### Microscopic foundations

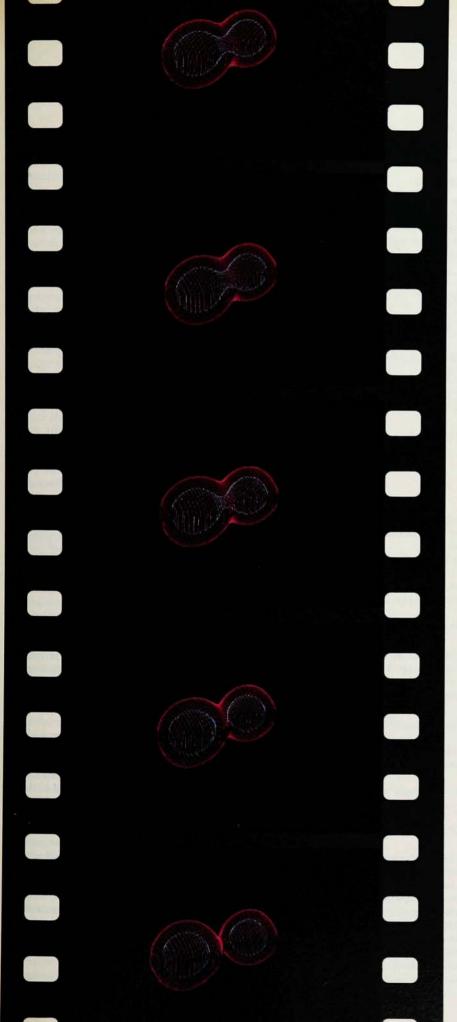
Although the nucleon-nucleon inter-

and gluon substructure of hadrons, one can describe the low-energy dynamics of nuclei-to within small corrections-in terms of a phenomenological two-body potential. A suggestive analogy is the interaction between helium atoms: The long-range attraction and short-range repulsion between two helium atoms, which can be derived from multiple photon exchanges and the interpenetration of electron clouds, are well represented by a phenomenological potential whose parameters are fitted to scattering data and measured virial coefficients. Similarly, for the nucleon-nucleon interaction, all the physics of meson exchange at large distances and overlapping bags of quarks at short distances is subsumed into a phenomenological potential. The strong short-range repulsion and intermediate-range attraction, the spin and isospin dependence, and the pronounced angular-momentum dependence of this potential are all made to fit physical information contained in scattering data and deuteron properties. The leading correction to this twobody-potential description in a nucleus arises from three-body processes, in which the internal degrees of freedom in a given nucleon are excited by interacting with one nucleon and deexcited by interacting with a different nucleon. Such processes only make a small correction to the dominant twobody physics and are described by three-body forces. Thus, like liquid helium, the nuclear many-body problem is essentially reduced to the study of a nonrelativistic quantum system interacting via very strong short-range

action ultimately arises from the quark

We now confront the essential ques-

John Negele is professor of physics at MIT; his research is in theoretical physics-specifically in many-body theory and nuclear structure.



Spontaneous fission. This sequence of density contours shows the spontaneous fission of a Be $^{8}$  nucleus into two  $\alpha$  particles; the outer and inner contours show the surfaces at which the density is  $^{1}\!\!/_{3}$  and  $^{2}\!\!/_{3}$  of the central density of the original Be $^{8}$  nucleus. The self-consistent computations for this process were performed on the Cray computer at the Los Alamos National Lab. The size of the systems that can be studied is at present limited by the capacity of the computer.

tion of the nonrelativistic nuclear many-body problem: Why should a self-bound system with strong shortrange interactions give rise to shell structure and be describable by a meanfield theory? The Hartree theory of an atom, in which the electrons propagate independently in a one-body mean field, is intuitively well motivated. First, there is a real, strong central field arising from the nuclear charge Z at the origin. Furthermore, because the electrons interact via a smooth, longrange force, it is plausible that the dominant effect of all the other electrons on a single electron is just the average one-body Coulomb potential they generate. Both of these features, however, are missing in a nucleus, so why should an independent-particle approximation based on a mean field still describe nuclear structure?

The answer lies in the Pauli exclusion principle. Most of the two-body scattering processes that could destroy the simple shell model are prohibited because the final states are already occupied by other nucleons. Only virtual excitations to high-energy unoccupied states are permitted. But because of the energy-time uncertainty relation, these excitations can only last a short time and are thus restricted to short distances. The net result is that the overall wavefunction must look very much like that of noninteracting particles in a one-body potential well, with little holes punched in it wherever any two particles get very close together and the Pauli principle permits the potential to induce strong two-body correlations.

The key to treating the strong nucleon interaction is thus calculating the short-range correlations in the

#### Path integrals

The Feynman path integral expresses the propagation of a single particle as an integral over trajectories in coordinate space. Mathematically, the expression is obtained by breaking the evolution for a time T into n steps of size  $\epsilon = T/n$ . For each step, one writes the unit operator in the form of an integral over a complete set of coordinate states  $1 = \int \mathrm{d}q |q\rangle \langle q|$  with the result.

Evaluation of the propagators  $\langle q_{k+1} | \mathrm{e}^{-iH\epsilon} | q_k \rangle$  for each infinitesimal time step then produces the familiar result

$$\begin{split} \langle q_t | \mathrm{e}^{-iHT} | q_i \rangle &= \int \mathrm{d}q_1 \dots \mathrm{d}q_n \mathrm{exp} \{ i\epsilon \sum_k [(m/2)(q_{k+1} - q_k)^2 / \epsilon^2 - V(q_k)] \} \\ &\to \int D[q(t)] \mathrm{exp} \Big\{ i \int S[q(t)] \Big\} \end{split}$$

where S is the classical action

$$S(q(t)) = \int_0^T \mathrm{d}t [(m/2)\dot{q}(t) - V[q(t)]]$$

and  $\int D[q(t)]$  is an integral over all possible paths q(t). The quantum propagator is thus expressed as the integral of the exponential of the classical action over all possible trajectories.

The propagator for N fermions may be expressed analogously as an integral over all possible trajectories in an appropriate space. We shall thus represent the unit operator at each time step not by  $\int \mathbf{d}q|q\rangle\langle q|$  but by an integral over an overcomplete set of Slater determinants

$$1 = \int D[\psi_m^*(\mathbf{r})\psi_n(\mathbf{r})]_{\mathrm{orthonormal}} |\Psi_{\mathrm{SD}}\rangle \langle \Psi_{\mathrm{SD}}|$$

Here,  $|\Psi_{\rm SD}\rangle$  is a completely antisymmetric linear combination of states of the form  $|\psi_a({\bf r}_1)\rangle|\psi_b({\bf r}_2)\rangle\cdots|\psi_f({\bf r}_N)\rangle$  and the appropriately normalized integral only extends over orthonormal functions. Evaluation of the propagators for each time step then yields the result

$$\langle \Psi_{\rm f} | {\rm e}^{-iHT} | \Psi_{\rm i} \rangle = \int D \big[ \psi_m^{\ *}({\bf r},t) \psi_n({\bf r},t) \big]_{\rm orthonormal} {\rm e}^{iS(\psi^*,\,\psi)}$$

where  $S(\psi^*, \psi)$  is the time-dependent Hartree–Fock action described in the text. Omitting exchange terms, we can write it as

$$\begin{split} S(\psi^*,\psi) &= \int \mathrm{d}t \bigg[ \int \mathrm{d}^3r \sum_m {\psi^*}_m(\mathbf{r}) [i(\partial/\partial t) + (1/2m)\nabla^2] \psi_m(\mathbf{r}) \\ &- \int d^3\mathbf{r} \mathrm{d}^3\mathbf{r}' \sum_{\mathbf{r},\mathbf{r}} {\psi^*}_m(\mathbf{r}) \psi^*_n(\mathbf{r}') \upsilon(\mathbf{r} - \mathbf{r}') \psi_m(\mathbf{r}) \psi_n(\mathbf{r}') \bigg] \end{split}$$

This functional integral provides a bridge between the quantum many-body propagator and the time-dependent Hartree–Fock action analogous to the Feynman path integral bridge between the quantum propagator and the classical action. In the stationary-phase approximation, the propagator between two Slater determinants is dominated by the exponential of a time-dependent Hartree–Fock solution, because the requirement that the action  $S(\psi^*,\psi)$  is stationary yields the time-dependent Hartree–Fock equation, and single-particle wavefunctions satisfying these equations are automatically orthonormal.

wavefunction. Two-particle correlations are determined by a scattering equation in which the nucleon-nucleon interaction between two particles is included explicitly; the remaining particles affect nucleon propagation via the mean field and the prohibition of scattering into states already occupied by other particles.2 One can systematically extend this formalism to n-body correlations by solving an analogous equation in which interactions between n particles are included explicitly and the remaining particles contribute via the mean field and Pauli exclusion principle. In effect, one is rearranging the perturbation series expansion in terms of correlations rather than powers of the (large) coupling constant. Detailed numerical calculations for bulk nuclear matter and light nuclei including two- and three-body correlations and estimates of four-body correlations yield3 two results crucial to the development of mean-field theory:

▶ The hierarchy of correlation terms converges sufficiently rapidly that the overwhelmingly dominant contributions come from two-body correlations. For these two-body correlations one can define an effective interaction, or pseudopotential, such that the matrix element of the true two-body interaction with the correlated wavefunction is equal to the matrix element of the effective potential with the uncorrelated single-particle wavefunction. Thus all the physics of two-body correlations can be included in an effective interaction to be used with simple uncorrelated single-particle wavefunctions. This effective interaction is strongly density dependent: As the nuclear density increases, more and more phase space is excluded by the Pauli exclusion principle, and the effective interaction must become less and less attractive. ▶ The density one calculates with all the many-particle correlations included is higher than one finds experimentally, although the binding energy of bulk matter is correct. To compensate for this, one introduces a small correction-at the level of a few percent of the total potential energy-from a three-

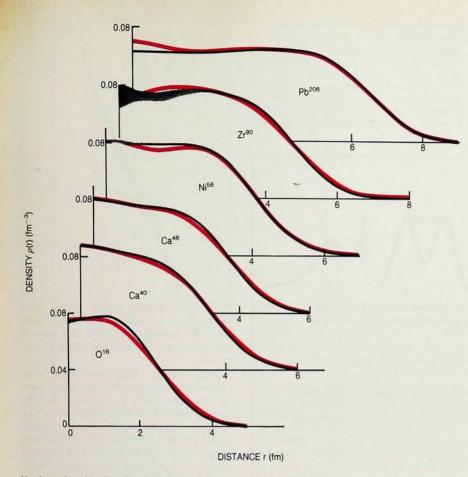
## The mean-field theory

dom.

We now have all the elements for the nuclear mean-field theory. The funda-

body potential to include the effect of

suppressed subnuclear degrees of free-



Nuclear density distributions. The graphs show a comparison of the theoretical (colored lines) and experimental (black lines) densities of six different spherical nuclei. The experimental values (shading indicates experimental uncertainty) are obtained from elastic electron scattering and muonic x-ray transitions; theoretical values are from mean-field calculations.

mental component is the effective interaction between nucleons. It is derived from the nucleon-nucleon potential and thus incorporates our full experimental knowledge of the nuclear interaction. It includes all the physics of two-body correlations-the little holes punched in the many-body wavefunction by strong, short-range forces. And it accounts for all but a small fraction of the total nuclear potential energy. To this microscopically derived effective interaction we add a small phenomenological density-dependent correction to account for threeand higher-body correlations and the three-body force. The two parameters in this correction are determined4 to fit the binding energy and equilibrium density of bulk matter. Although the derivation of the total effective interaction involves technically complicated numerical calculations, the final result is essentially state independent and may be represented<sup>4,5</sup> in an extremely simple and tractable form.

To derive the effective equations of motion, we start with a quantum analog of Hamilton's principle, namely that the action

$$S = \int dt \langle \Psi | i \frac{\partial}{\partial t} - H | \Psi \rangle$$

is a stationary quantity. The wavefunction  $\Psi$  is the complete wavefunction of all nucleons in the nucleus. Because nucleons are fermions, this wavefunction must be completely antisymmetric in the variables for identical particles. We can account for this by writing the uncorrelated wavefunction as a Slater determinant of singleparticle wavefunctions  $\psi_k(\mathbf{r})$ , that is, as a sum of products  $\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)...\psi_f(\mathbf{r}_N)$ completely antisymmetrical with respect to the coordinates  $\mathbf{r}_1, \dots \mathbf{r}_N$ . We obtain the mean-field approximation by replacing Ψ in the action by a Slater determinant and by replacing the twobody interaction in H by the densitydependent effective interaction  $v_{\rm eff}$ . This yields the action  $S(\psi^*, \psi)$  discussed in the box on the opposite page.

The action integral thus becomes a functional of the wavefunctions  $\psi_k(\mathbf{r})$ , which play the role of canonical coordi-

nates in this Hamiltonian formalism; the conjugate momenta are the conjugate wavefunctions  $i\psi_k^*(\mathbf{r})$ . Requiring the action S to be stationary with respect to variations in the wavefunctions  $\psi$  yields, as in the classical Hamiltonian formalism, equations of motion. In this case, they are the time-dependent Hartree–Fock equations

$$\begin{split} i \, \frac{\partial}{\partial t} \, \psi_k(\mathbf{r}, t) \\ &= - (1/2m) \nabla^2 \psi_k(\mathbf{r}, t) \\ &+ \big[ \int \mathrm{d}^3 r' v_{\text{eff}}(\mathbf{r}, \mathbf{r}') \Sigma_m \psi_m \,^*(\mathbf{r}', t) \psi_m(\mathbf{r}', t) \big] \\ &\times \psi_k(\mathbf{r}, t) \end{split}$$

I have simplified these equations somewhat by omitting the density dependence of  $v_{\rm eff}$  and the exchange terms. Actual calculations, of course, include both.

These equations describe a time-dependent mean-field theory in which each single-particle wavefunction evolves in the self-consistent field generated by all the other nucleons interacting via the effective interaction. As the total wavefunction  $\Psi$  changes its spatial distribution, the evolution of the little holes punched in it by strong short-range forces is taken into account through the density dependence of the effective interaction.

## Static solutions

The first quantitative test of the theoretical ideas I have described is to calculate the gross ground-state properties of finite nuclei. For this we need stationary solutions to the time-dependent Hartree-Fock equations, that is, solitons of the form

$$\psi_m(\mathbf{r},t) = e^{-i\epsilon_m t} \phi_m(\mathbf{r})$$

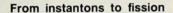
In that case, the wavefunctions  $\phi(\mathbf{r})$  satisfy a self-consistent eigenvalue problem:

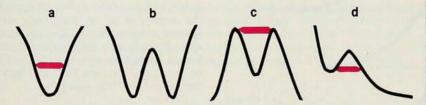
$$[-(1/2m)\nabla^2 + V(\mathbf{r})]\phi_m(\mathbf{r}) = \epsilon_m \phi_m(\mathbf{r})$$

where the self-consistent potential is

$$\label{eq:V} V\!(\mathbf{r}) = \int \mathrm{d}^3r' \upsilon_{\mathrm{eff}}(\mathbf{r} - \mathbf{r}') \sum_m \! \phi_m^*(\mathbf{r}') \phi_m(r')$$

Solutions of these equations yield excellent quantitative agreement with observed nuclear properties throughout the periodic table. Binding energies are typically reproduced to within 0.3 MeV per particle out of a total potential energy per particle of 40





One simple way to study the quantum spectrum of a particle in a potential is to find the poles in the trace of the propagator using a Feynman path integral

$$\sum_{n} \frac{1}{E-E_n+i\eta} = tr \frac{1}{E-H+i\eta} = i \int_0^\infty \mathrm{d}T \, \mathrm{e}^{iET} \int \mathrm{d}q \int D[q(t)] \, \mathrm{e}^{iS(q(t))}$$

If we apply the stationary-phase approximation to each of the three integrals in the last expression, the result is given by the sum of the exponentials of the classical action for all periodic trajectories having classical energy *E*.

For a single well of the form shown in sketch a above, periodic trajectories satisfying the classical equations

$$m\,\frac{\mathrm{d}^2q}{\mathrm{d}t^2} = -\,\nabla\,V(q)$$

correspond to the motion of a marble rolling in a valley described by V(q). A continuum of such periodic solutions exists, and in lowest approximation the sum over classical solutions produces poles at those energies for which a periodic trajectory has an action satisfying the Bohr–Sommerfeld condition

$$2\pi n = \oint p\dot{q}dt$$

When the integral over fluctuations is included,  $2\pi n$  is replaced by the familiar factor  $(2n + \frac{1}{2})\pi$ .

Now consider periodic solutions connecting the left and right minima in the double well shown in sketch  ${\bf b}$ . Clearly, for energies below the top of the barrier there are no such periodic classical solutions: The marble will roll down one of the valleys and oscillate around the corresponding minimum. However, in performing the time integral in the path integral above using the method of steepest descent, one is obliged to seek stationary solutions for all values of T in the complex plane. For purely imaginary time, we may rewrite the equations in terms of a real variable  $\tau=it$  so that the equation of motion involving two time derivatives acquires an overall minus sign; we can group this minus sign with the potential:

$$m\frac{\mathrm{d}^2q}{\mathrm{d}\tau^2} = -\nabla[-V(q)]$$

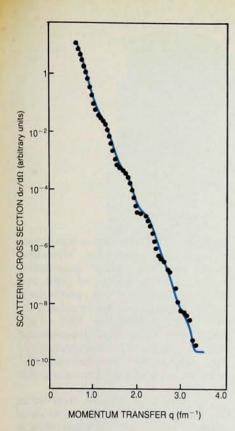
Thus stationary solutions for imaginary time correspond to classical solutions in an inverted potential, as shown in sketch  $\mathbf{c}$ . For the case of the double well with two equally deep minima, the classical solutions corresponding to a marble rolling from the top of one hill, across the valley, and up to the top of the other hill has come to be known as an instanton. Such periodic imaginary-time solutions exist in any potential having a classical forbidden regime, and for example, the lifetime of a metastable state in the potential shown in sketch  $\mathbf{d}$  is given by such a solution connecting the relative minimum to the outside of the barrier. The generalization of this argument to the many-fermion problem provides a microscopic theory of spontaneous fission.

MeV, and charge radii agree with experiment to within 0.05 fm. Thus both the potential energy and spatial extent are accurate to the order of one percent.

High-energy, high-resolution electron scattering provides stringent tests of the mean-field predictions for the spatial distribution of charge in the nucleus. Figure 2 shows the predicted4 radial charge densities for six spherical nuclei. Note that the nuclei all have a roughly constant interior density, modulated by density fluctuations arising from single-particle shell structure, and a surface layer in which the density falls off in the same way for all the nuclei. The quantitative predictive power of the theory is demonstrated in figure 3, which shows a comparison7 of the scattering cross section of Pb208 for elastic electron scattering as calculated using the mean-field density and as subsequently measured. The agreement is good over 11 orders of magni-

One can invert<sup>5</sup> elastic-scattering data to determine the charge distribution of the nucleus. If the data extend to sufficiently large momentum transfer, the density is given with high precision. Figure 2 also shows such experimentally derived charge distributions; the agreement between the mean-field calculations and experiments is clearly good throughout the periodic table.

A significant manifestation of the interplay between single-particle and collective degrees of freedom in nuclei is the fact that nuclei in several regions of the periodic table are intrinsically deformed. Like a diatomic molecule, a well-deformed nucleus has an entire band of rotational states built upon a single intrinsic state. By measuring the elastic and inelastic scattering to each state in the ground-state rotational band, one can determine the radial functions for each term in the Legendre expansion of the deformed



Elastic electron scattering from lead-208. The solid curve shows a plot of scattered intensity as a function of momentum transfer as derived from mean-field calculations; the experimental points were obtained from the scattering of 502-MeV electrons at Saclay. The excellent agreement confirms the predicted radial charge distribution in lead.

intrinsic state and thus determine the precise shape of the deformed nucleus.

A significant quantitative success of the mean-field theory has been its ability to predict correctly which heavy nuclei are spherical and which are deformed, and what the shapes of the deformed nuclei are. The addition of only a few neutrons is enough to tip the balance between spherical and aspherical, and the mean field manifests this sensitivity in correctly predicting,8 for example, Sm148 to be spherical and Sm152 to be well deformed. Figure 4 shows another example of the predictive power of the theory, in this case for electron scattering to the lowest four rotational states in the ground-state band of U238; the theoretical curves8 are based on the deformed intrinsic state of U238, whose shape was calculated before the precise high-resolution experimental data9 shown in the figure were available.

# From nuclei to neutron stars

The quantitative success of the mean-field theory for terrestrially observed nuclei provides us with a basis for extrapolating it to nuclear strucFigure 4

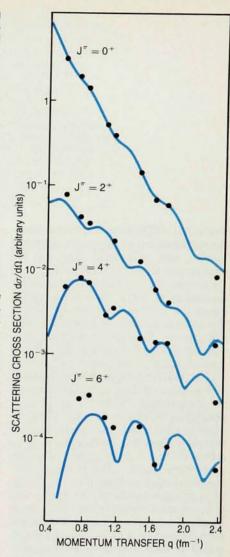
Elastic and inelastic electron scattering from uranium-208. The U<sup>208</sup> nucleus is aspherical, so the ground state has a band of rotational states, which can be excited by electron scattering. The data come from the energy-loss spectrometer at the MIT Bates accelerator. The agreement confirms our understanding of the shape of this highly deformed nucleus.

Figure 4

tures that may arise elsewhere in the universe under experimentally inaccessible conditions. One such example is the baryonic matter in a neutron star. As a heavy star collapses under its own gravitational field, it becomes energetically favorable for more and more of the protons and electrons to combine to form neutrons: The Fermi energy of an electron in a Fermi gas increases so much with increasing density that it exceeds the nuclear energy required to increase the ratio of neutrons to protons. If the temperature of the star is below 108 K (corresponding to a negligible 10 KeV on the nuclear energy scale) and the density is below 1.6×10<sup>36</sup> baryons/cm<sup>3</sup>, all the conditions for the validity of the mean-field theory are satisified. We can thus use the theory to investigate the behavior of neutron stars.

Figure 5 shows the sequence of nuclei calculated10 to occur in a chunk of neutral matter as its density is increased from roughly 0.1% of the typical nuclear-matter density to 1/3 nuclear density. The material starts as a block of terrestrially observed Zr90; as it is compressed, the nuclei become successively more neutron rich, until neutrons eventually drip out of the nuclei, forming a low-density neutron gas in the intervening space. Eventually, as the density of the block approaches nuclear densities, the matter distribution becomes uniform and is composed primarily of neutrons with a small component of protons. The study of neutron-star matter at subnuclear densities has important implications for the equation of state of dense matter, for the composition and observable properties of the crusts of neutron stars, and for supernova collapse.

Other terrestrially inaccessible conditions govern the burning of nuclei in the Sun and other stars and determine the abundance of heavy elements produced by supernovae. These applications of the theory are at the frontier



for fruitful interplay between nuclear many-body theory and astrophysics.

## Time-dependent problems

The physical ideas embodied in the self-consistent calculations I have described are clearly useful in understanding the nuclear ground state. To apply these ideas to large-amplitude collective motion and low-energy nuclear dynamics, we must return to the time-dependent Hartree-Fock equation. The mean field contains all the relevant information about shape and hydrodynamic degrees of freedom built into familiar collective models. Furthermore, the time-dependent meanfield theory is completely self-contained, with the collective variables and their dynamics being fully specified by the nuclear Hamiltonian and the physical process under consideration.

The equations of motion for the single-particle wavefunctions  $\psi_k(\mathbf{r},t)$  specify a classical Hamiltonian field theory of immense richness and complexity. They allow us to follow the evolution of nuclear wave packets through collisions or reactions. For the

moment, I will defer questions concerning semiclassical aspects of the approximation and will focus first on its application to nuclear collisions.

Consider the collision of two nuclei at an energy of a few MeV per particle above the Coulomb barrier, for which the approximations we have discussed make sense. The initial condition for a nuclear collision is given by taking ground states of the target and projectile approaching each other with specified relative velocity and relative angular momentum. There is no known analytical technique to even begin to analyze such highly nonlinear coupled integro-differential equations, so one solves them numerically on a discrete space-time mesh. The scale of the computational problem is at the limits of existing computers: For heavy nuclei, one must compute the values for a hundred or more complex functions. each defined on a mesh having tens of points in each of three spatial dimensions, for hundreds of time steps.

Figure 6 shows the calculated11 results for two typical nuclear collisions. The first sequence of contour plots, on page 32, shows the evolution of the density for a peripheral collision between O<sup>16</sup> and Ca<sup>40</sup> at a laboratory energy of 315 MeV. Each picture shows the integrated density normal to the reaction plane seen in the center-ofmass frame. The oxygen nucleus approaches from the right and the calcium nucleus approaches from the left. They are separated by a large impact parameter, corresponding to a relative angular momentum of 80%, so that they overlap only slightly as they pass through each other. Nevertheless, the final fragments are very different from the initial ground states. In addition to the significant distortion of the density visible in the figure, many nucleons have been transferred between the two nuclei, and much of the initial collective translational kinetic energy has been converted into internal excitation energy.

Just how dramatic the nonlinear collective effects can be is shown in the other sequence of figure 6. This collision is slightly more head-on. The

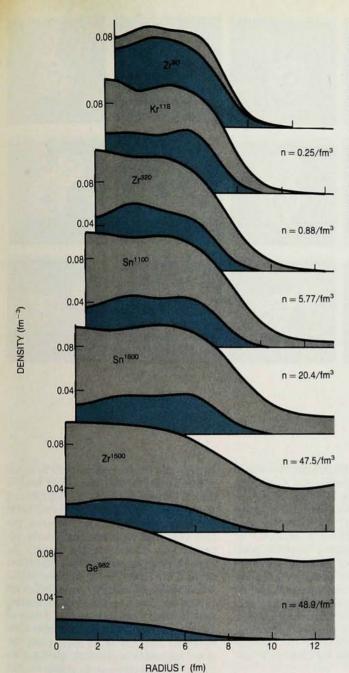
nuclei now have a relative angular momentum of 60%. Instead of grazing each other, the nuclei fuse together and form a single compound nucleus. All of the collective translational kinetic energy is transferred into single-particle degrees of freedom. The time-dependent Hartree-Fock theory is rich enough that an infinitesimal change in a continuous variable specifying the initial condition—in this case the relative angular momentum-gives rise to a discontinuous change in qualitative behavior-in this case the transition from fission to fusion. To complement the large-scale numerical calculations. we have gained a significant insight into the way complex physics comes12 from single-particle behavior by physical arguments and studies of simplified geometries.

There are two important experimental tests of this mean-field description of nuclear dynamics: the systematics of fusion cross sections and the energy loss in deep-inelastic collisions. The fusion cross section in the time-dependent Hartree-Fock approximation is given by a semiclassical expression that involves a sum over all relative angular momenta for which the target and projectile fuse. Figure 7 shows the results of mean-field calculations13 for the fusion of O16 + O16 at a variety of bombarding energies as well as results of experimental measurements14 of the fusion cross section. The theory reproduces quantitatively the effects of energy dissipation from collective to singleparticle degrees of freedom over a wide range of bombarding energies. At the lowest energies, the theory correctly describes the transition from widely separated Coulomb trajectories for which the nuclei never overlap to configurations like the nearly head-on collision shown in the sequence on page 33, in which sufficient dissipation occurs to cause fusion. The theory continues to match the experimental data for high energies despite a change in behavior: Although increasingly many values of the angular momentum correspond to substantial overlap at the highest energies, the relative velocities become so high that for many angular momenta the dissipation is insufficient to make the system fuse. Mean-field theory has had similar quantitative successes for a variety of light and intermediate nuclei. A particularly striking example is the calculated fusion cross section for  $\operatorname{Ca^{40}} + \operatorname{Ca^{40}}$ , which was in serious disagreement with the then-available experimental data; subsequent remeasurements, however, showed good agreement with the theory.

The large energy losses observed in what have come to be known as deepinelastic heavy-ion collisions were a great surprise to nuclear experimentalists: Over a wide range of kinematical conditions, many of the collision fragments in a heavy-ion collision correspond to nuclei with roughly the masses of the target and projectile, but with such high excitation energies that almost all of the original translational kinetic energy is converted into internal excitation energy. Again, the evolution of single-particle wavefunctions in the mean-field approximation provides the microscopic explanation for this pronounced dissipation. Quantitative comparison with experiment for deep-inelastic scattering of heavy nuclei, such as  $Kr^{84} + Bi^{209}$  or  $Xe^{136} + Bi^{209}$ , is more difficult than the evaluation of light-ion fusion cross sections, both because of the semiclassical nature of the time-dependent Hartree-Fock approximation and because computational limitations necessitate additional physical approximations for very large systems. Nevertheless, the time-dependent mean-field calculations have successfully accounted for 80-100% of the energy dissipation observed experimentally in a variety of heavy-ion collisions.

## Path integrals and the mean field

Although the time-dependent Hartree-Fock theory embodies a great deal of the physics of nuclear dynamics, it is limited by its semiclassical character. As it stands, it is not clear how to use it to calculate quantized eigenstates of collective vibrations, how to calculate a quantum-mechanical differential cross section, or how to treat the quantum-



Nuclear matter in neutron stars. The progression of graphs shows the calculated density of neutrons (black) and protons (color) as a chunk of material is squeezed to successively higher densities. The material starts out as terrestrial Zr90, at 0.1% of nuclear density, or 2.5 × 1035 baryons/cm3. As the material is compressed, the Fermi energy of the electrons surrounding the atoms becomes so large that it is energetically favorable for some of them to combine with protons to form neutrons. Eventually neutrons drip out of the nuclei to form a gas. For the highest density shown, roughly 1/3 of nuclear density, there are about 30 neutrons for each proton. Figure 5

mechanical tunneling that arises in spontaneous fission. Having already seen how the static mean-field theory can be understood as the first step in a systematic sequence of approximations in quantum many-body perturbation theory, we now seek a corresponding quantum mechanical framework for understanding the time-dependent

mean-field theory.

A beautiful and powerful physical framework for such an understanding is provided by path integrals. As summarized in the box on page 26, the Feynman path integral<sup>15</sup> for a single particle in a potential expresses the quantum amplitude for propagating from an initial state with a particle at position  $q_i$  to a final state with the particle at  $q_f$  as an integral over an exponential containing the classical

action

$$egin{aligned} \langle q_t | \mathrm{e}^{-iHT} | q_i 
angle \ &= \int \!\! D[q(t)] \! \exp \! \left\{ i \! \int_0^T \! \mathrm{d}t S[q(t)] 
ight\} \end{aligned}$$

A useful approximation is obtained from the familiar stationary-phase approximation. The dominant contribution to the integral comes from that trajectory q(t) for which the action is stationary. But variation of the action S[q(t)] just yields the classical motion for a particle in the potential, so the dominant contribution is proportional to  $e^{iS[\varphi(t)]}$  where  $\varphi(t)$  is the classical trajectory for a particle propagating from  $q_i$  to  $q_f$  in time T. Systematic corrections to this classical approximation are obtained by expanding S[q(t)]around the classical solution q(t) and

performing the resulting integral over the fluctuations  $q(t) - \varphi(t)$ . The crucial feature for our present purpose is the fact that the leading term in a systematic quantum theory is given by classical equations obtained from the condition that the classical action is stationary.

There are several essentially equivalent ways to derive an analogous functional integral for the many-fermion problem; these make use of an auxiliary field, fermion coherent states, or overcomplete sets of Slater determinants. Because of its similarity to the Feynman path integral, I outline the method using Slater determinants6 in the box on page 26.

The features of the theory, which are derived17,18 in detail in the literature, are intuitively plausible generalizations of the single-particle theory. In summary, the correspondence between the single-particle and many-fermion

results is as follows:

► The integral of e<sup>iS</sup> over all paths in coordinate space is replaced by an integral of eis over all paths in the space of Slater determinants.

▶ The time-dependent Hartree-Fock action  $S[\psi^*(\mathbf{r},t),\psi(\mathbf{r},t)]$  replaces the clas-

sical action S[q(t)].

▶ The canonically conjugate fields  $\psi(\mathbf{r},t)$  and  $i\psi^*(\mathbf{r},t)$  correspond to the classical coordinate q and the conjugate momentum p.

▶ In the stationary-phase approximation, the action is dominated by solutions to the time-dependent Hartree-Fock equations instead of the classical

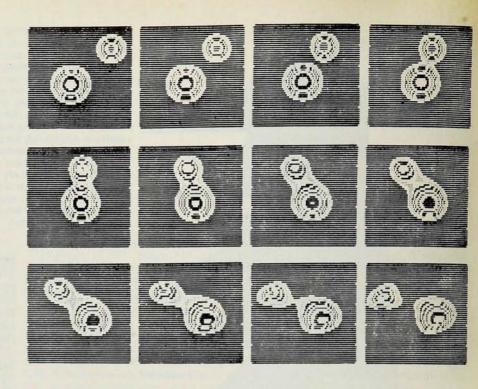
trajectory

 Quantized eigenstates are given by periodic solutions to the time-dependent Hartree-Fock equations with an orthonormalization constraint rather than by periodic classical trajectories; the quantization condition

$$\int dt d^3r \sum_m i \psi_m^*(\mathbf{r}, t) \partial \psi_m(\mathbf{r}, t) / \partial t$$

replaces the Bohr-Sommerfeld condition

$$\int \! \mathrm{d}t \, p(t) \, \mathrm{d}q(t) / \mathrm{d}t = 2\pi n$$



▶ Tunneling solutions in classically forbidden regions are obtained by replacing it by the real variable  $\tau$  as in the one-particle case.

The equations for quantized eigenstates, again written without exchange terms for simplicity, pose the following self-consistent eigenvalue problem in four space-time dimensions<sup>17</sup>

$$\begin{split} [\; -i\partial/\partial t - (1/2m)\nabla^2 + V(\mathbf{r},t)] \psi_m(\mathbf{r},t) \\ = \lambda_m \psi_m(\mathbf{r},t) \end{split}$$

$$\begin{split} V(\mathbf{r},t) &= \int \! \mathrm{d}^3 r' v(\mathbf{r} - \mathbf{r}') \sum_n \! \psi_n \, ^*(\mathbf{r}',t) \psi_n(\mathbf{r}',t) \\ \psi_m(\mathbf{r},t) &= \psi_m(\mathbf{r},0) \end{split}$$

Note that these equations are analogous in structure to the static Hartree–Fock eigenvalue problem I described earlier, but these contain an extra time variable. One may think of the parameters  $\lambda_m$  as Lagrange multipliers enforcing the orthonormality of the wavefunctions  $\psi^*$  and  $\psi$  required in the functional integral. By using suitable iterative techniques, one can find solutions to these equations for a continuum of values of the period T; the quantum eigenstates are specified by the discrete values of T such that

$$\int_{o}^{T} \mathrm{d}t \int \mathrm{d}^{3}\mathbf{r} \sum_{m} i \psi_{m}^{*} \partial \psi_{m} / \partial t = 2\pi n.$$

In the limit in which each  $\psi_m(\mathbf{r},t)$  differs only infinitesimally from the static Hartree–Fock solution  $\psi_m(\mathbf{r})$ , these equations reduce<sup>17</sup> to the familiar

random-phase approximation, which has proved to be extremely successful in describing a broad range of smallamplitude collective phenomena in nuclei. For example, the same level of quantitative precision is obtained in predicting the inelastic electron scattering to collective excited states in Pb<sup>208</sup> as that shown in figure 3 for the ground state. For large-amplitude collective motions, these equations provide the only theory currently available that does not require additional adiabatic assumptions or the imposition of prescriptions for collective variables.

#### Spontaneous fission

The box on page 28 shows how to extract the quantum mechanics of a single particle moving the classically forbidden region of a potential from the Feynman path integral by considering stationary points in the action corresponding to imaginary time. A picturesque way to think about the two factors of i in the equation of motion arising from the replacement  $it \to \tau$  is to consider the classical motion in the inverted potential -V(q).

The idea that such imaginary-time solutions may dominate the action in certain circumstances, first introduced<sup>19</sup> in the study of bubble formation, provides a foundation for the theory of spontaneous fission. Several technical points arise in the course of the derivation that are not obvious from the analogy presented here. It

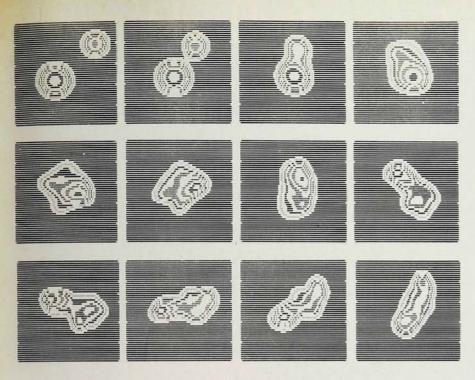
turns out that the appropriate analytic continuation of the conjugate field is  $\psi(\mathbf{r},t^*)^*$  so that the fields  $\psi^*(\mathbf{r},t)$  and  $\psi(\mathbf{r},t)$  are replaced by new fields  $\psi(\mathbf{r}, -\tau)$  and  $\psi(\mathbf{r}, \tau)$ . Furthermore, the fact that the relevant many-body potential has been inverted is only obvious if one transforms from the fields  $\psi^*$  and  $\psi$  to their modulus and phase. The final result is that the contribution to the action governing the tunneling between the metastable ground state of a fissile nucleus and a particular open reaction channel with separating fission fragments is given by the solution to the self-consistent equation

$$\begin{split} [\partial/\partial\tau - (1/2m)\nabla^2 + V(\mathbf{r},\tau)] \bar{\psi}_m(\mathbf{r},\tau) \\ &= \tilde{\lambda}_m \bar{\psi}_m(\mathbf{r},\tau) \\ V(\mathbf{r},\tau) &= \int \!\!\!\mathrm{d}^3r' v(\mathbf{r}-\mathbf{r}') \\ &\times \Sigma_n \bar{\psi}_n(\mathbf{r}',-\tau) \psi_n(\mathbf{r}',\tau) \\ \bar{\psi}_n(\mathbf{r},T) &= \bar{\psi}_n(\mathbf{r},0) \end{split}$$

Given a solution to these equations for each reaction channel c, the inverse lifetime is a sum over partial widths for each reaction channel

$$\begin{split} \Gamma &= \Sigma_c \lim_{T \to \infty} \Gamma^{(c)}(T) \\ \Gamma^{(c)}(T) &= K \exp \bigg[ - \int_{-T/2}^{T/2} \mathrm{d}\tau \int \mathrm{d}^3 r \\ &\times \sum_m \tilde{\psi}_m(\mathbf{r}, -\tau) \frac{\partial}{\partial \tau} \, \tilde{\psi}_m(\mathbf{r}, \tau) \bigg] \end{split}$$

The factor K is obtained from integrating quadratic fluctuations around the stationary solution. Since  $\psi(\tau)$  and



Collision between O<sup>16</sup> and Ca<sup>40</sup>. The sequence of contour plots on the opposite page shows a grazing collision: The impact parameter is nearly the sum of the nuclear radii (the relative angular momentum is 80ħ); nonetheless, a considerable amount of distortion and excitation results. In the sequence shown at left, on this page, the impact parameter is slightly smaller (the relative angular momentum is 60ħ), and the collision results in fusion of the nuclei.

 $\psi(-\tau)$  now play the role of coordinates and momenta, the expression for  $\Gamma$  has a form like that resulting from the Wenzel-Kramers-Brillouin method

$$\Gamma = \frac{\omega}{2\pi} \exp \left[ -\oint \! \mathrm{d}t \, p \dot{q} \, \right]$$

The self-consistent wavefunction evolves from the metastable ground state of the parent nucleus, through a classically forbidden region, to a point at which two just-separated daughters have reentered the classically allowed region. Figure 8 shows this process18 for a one-dimensional nucleus containing 16 particles. The graphs show density profiles at successive values of the imaginary time  $\tau$ , starting with the ground-state density of the parent, and concluding with the final, classically allowed state in which the system has nearly separated into two eight-particle clusters.

Applying these ideas to realistic nuclei is limited thus far by the computational scope of the problem. One must solve a set of coupled self-consistent integro-differential space-time equations; a heavy nucleus requires up to a hundred wavefunctions defined on tens of mesh points in each of four spacetime dimensions. The first solution of the tunneling equations for a physical system having nontrivial space-time geometry is a prototype calculation1 of the fission of Be8 into two a particles. The results are shown in figure 1. The calculation demonstrates the ability of the theory to select the relevant shapes and collective degrees of freedom that dominate the action. Once we can apply it to heavy fissile nuclei, this theory will provide the first microscopic quantum framework that takes into account the bulk liquid-drop behavior, the collective dynamics and the single-particle effects to which fission observables are known to be extremely sensitive.

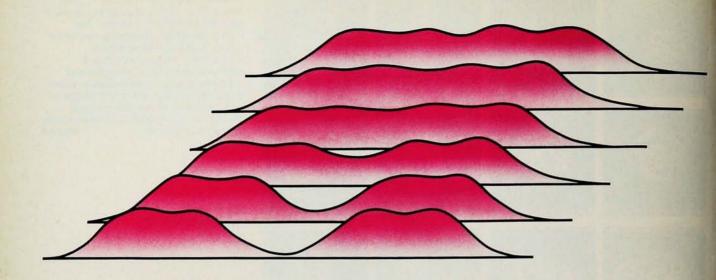
## **Nuclear partition function**

Evaluating the many-fermion path integral in imaginary time also provides a means to calculate  $^{20}$  the nuclear partition function  $Z=tr\,({\rm e}^{-\beta H})$ . The nuclear system to which quantum statistical mechanics is clearly relevant is the hot equilibrated baryon matter in neutron stars. The mean-field approximation provides an obvious generalization of the zero-temperature Hartree-Fock approximation. By weighting each single-particle state with a thermal occupation factor, one can use the theory to provide a framework for calculating observables of astrophysical interest such as the level density and equation of state of neutron-star matter at finite temperature.

The finite-temperature theory has also been used to obtain an approximation to the nonequilibrium statistical mechanics of compound nuclei. The excited compound nuclei created in nuclear reactions decay by photon and particle emission; their statistical behavior during this process indicates a high degree of equilibration. One can

make use of this thermal equilibrium to find approximate descriptions of induced fission<sup>20</sup> and the statistical properties of highly excited nuclei.<sup>21</sup> The finite-temperature mean-field theory allows one to find the properties of a box containing a hot nucleus in equilibrium with a low-density nucleon gas; after subtracting the background contribution of the low-density gas, one has an approximation to the compound nucleus.

The applications of nuclear meanfield theory I have surveyed suggest the range of phenomena that it can explain microscopically and indicate the quantitative precision it can provide. But these achievements should not obscure the remaining open challenges. Although we know how to calculate simple observables such as the fission lifetime, and although we have made some progress22 in approximating transition amplitudes, we have yet to work out a practical formulation of scattering theory that allows one to calculate such interesting observables as inclusive cross sections, fusion probability in subbarrier heavy-ion reactions, or the cross sections for forming superheavy nuclei. Substantial formal questions remain, such as understanding the range of validity of the stationaryphase approximation and properly embedding the effective interaction in the path-integral formulation. There are as well the formidable computational problems that I have mentioned. Looking beyond nuclear physics, small drops



**Nuclear fission.** The graphs show a sequence of density profiles representing the most probable path for the fission of a hypothetical 16-particle, one-dimensional nucleus. This mean-field result for the many-body problem is analogous to the instanton described in the box on page 28.

Figure 8

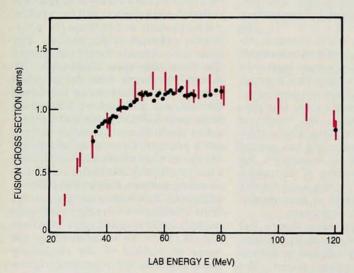
of liquid He<sup>3</sup>, He<sup>4</sup> and noble gases will pose a broad range of related problems when experimental techniques are developed to observe them. Many challenges remain in fully understanding the physics of small drops of dense, strongly interacting quantum physics.

#### References

- Extensive references to the work surveyed in this article are given in J. W. Negele, Rev. Mod. Phys. 54, 913 (1982).
- K. A. Brueckner, C. A. Levinson, Phys. Rev. 97, 1344 (195).
   K. A. Brueckner, Phys. Rev. 97, 1353 (1955); 100, 36 (1955).
   H. A. Bethe, J. Goldstone, Proc.

- R. Soc. Lond. A238, 551 (1957). L. C.
  Gomes, J. D. Walecka, V. F. Weisskopf,
  Ann. Phys. (N.Y.) 3, 241 (1958); H. A.
  Bethe, Phys. Rev. B138, 804 (1965).
- B. D. Day, Rev. Mod. Phys. 50, 495 (1978); H. K. Kümmel, K. Lührmann, J. Zabolitsky, Phys. Rep. C36, 1 (1978).
- J. W. Negele, D. Vautherin, Phys. Rev. C 5, 1472 (1972); J. W. Negele, Phys. Rev. C 1, 1260 (1970); D. Gogny in, Nuclear Self-Consistent Fields, G. Ripka, M. Porneuf, eds., North-Holland, Amsterdam (1975), p. 33.
- J. L. Friar, J. W. Negele, Adv. Nucl. Phys. 8, 219 (1975).
- A. K. Kerman, S. E. Koonin, Ann. Phys. (N.Y.) 100, 322 (1976).

- B. Frois, et al., Phys. Rev. Lett. 38, 152 (1977).
- J. W. Negele, G. Rinker, Phys. Rev. C 15, 1499 (1977).
- C. Creswell, PhD dissertation, Massachusetts Institute of Technology (1977).
- J. W. Negele, D. Vautherin, Nucl. Phys. A207, 298 (1973).
- M. S. Weiss, Fizika 9, Suppl. 3, 315 (1977).
- P. Bonche, S. E. Koonin, J. W. Negele, Phys. Rev. C 13, 1226 (1976); G. F. Bertsch, in Nuclear Physics with Heavy Ions and Mesons, Les Houches Summer School XXX, R. Balian, M. Rho, G. Ripka, eds., North-Holland, Amsterdam (1978).
- P. Bonche, B. Grammaticos, S. E. Koonin, Phys. Rev. C 17, 1700 (1978).
- M. Conjeaud, et al., in Proc. Int. Conf. on Nuclear Structure, Tokyo, September 1977, International Academic Printing Co., Japan (1977) p. 663
- R. P. Feynman, A. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, New York (1965).
- H. Kuratsuji, T. Suzuki, Phys. Lett. B92, 19 (1980); J. P. Blaizot, H. Orland, Phys. Rev. C 24, 1740 (1981).
- S. Levit, J. W. Negele, Z. Paltiel, Phys. Rev. C 21, 1603 (1980); H. Reinhardt, Nucl. Phys. A346, 1 (1980).
- S. Levit, J. W. Negele, Z. Paltiel, Phys. Rev. C 22, 1979 (1980); H. Reinhardt, Nucl. Phys. A367, 269 (1981).
- J. Langer, Ann. Phys. (N.Y.) 54, 258 (1969).
- A. K. Kerman, S. Levit, Phys. Rev. C 24, 1029 (1981).
- P. Bonche, S. Levit, D. Vautherin, Nucl. Phys. A427, 278 (1984); A436, 265 (1985).
- S. Levit, Phys. Rev. C 21, 1594 (1980); Y. Alhassid, S. E. Koonin, Phys. Rev. C 23, 1590 (1981); R. Balian, M. Vénéroni, Phys. Rev. Lett. 47, 1353 (1981).



Cross sections for the fusion of colliding oxygen nuclei as a function of the bombarding energy. The mean-field predictions (color) clearly account for the main features of the data (black), in particular, for the dissipation of energy from collective to single-particle degrees of freedom.

Figure 7