Model for tunneling in many-particle systems

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A model is proposed for studying tunneling in many-particle systems that is simple enough to solve and realistic enough to test various collective models of multidimensional barrier penetration. We find that the imaginary time dependent mean-field theory works very well in its domain of applicability, as does a continuum hopping approximation. The usual cranked mean field approximation is much less reliable.

I. INTRODUCTION

Tunneling in many-particle systems is an interesting problem with application in nuclear physics to spontaneous fission, exotic radioactivity, band mixing in deformed nuclei, as well as in heavy ion fusion reactions. A number of methods have been developed to treat the dynamics in the classically forbidden domain, but for the most part the techniques are of unproven reliability. All microscopic theory starts from a mean field or mean-field wave functions, but the symmetry of these wave functions must be broken in the barrier penetration. In one kind of theory, the symmetries are broken by the pairing interaction, which then provides the dynamics of the tunneling. On the other hand, in the imaginary time mean-field theory, the residual interaction is treated as a fluctuating mean field, which accomplishes the same effect. We would like to understand better whether these mechanisms are different ways of expressing the same physics, or whether there are intrinsic differences.

In this work we propose a model to test the various methods of treating large amplitude collective motion. The requirements of the model are first that it be simple enough so the solution can be found to whatever accuracy is desired. In order to be physically interesting, the model should have a continuous coordinate, to simulate the continuous dependence of the single particle wave function on position. The model also needs to have multiple isolated Hartree minima to mimic the physical situation in solving the fermion Hartree problem. This we achieve by augmenting the variables in the wave function to include a discrete variable which represents in some way the different symmetry states in the coordinates transverse to the z coordinate.

To provide a model of barrier penetration, the energies of the Hartree states of the Hamiltonian should be low in two distinct regions of configuration space. These should be separated by a barrier region with high Hartree energies, so that tunneling physics will apply to the low eigenstates. Finally, the Hamiltonian needs to have a residual interaction that breaks the Hartree symmetries, and allows the wave function to spread over the entire space of configurations. We have found a model to meet these goals, constructed as follows. The Hamiltonian governs the dynamics of N distinguishable particles. Each of these has a z coordinate as well as an internal spin coordinate. The Hamiltonian consists of an oscillator one-body part together with a two-body interaction that couples the z coordinate to the spin. Specifically, we define the Hamiltonian as

$$H=\sum_{i=1}^{N}\frac{1}{2}\left[-\frac{d^2}{dz_i^2}+z_i^2\right]+\kappa\left[\sum_{i=1}^{N}z_i\right]\left[\sum_{i=1}^{N}\sigma_z(i)\right]+\lambda\left[\sum_{i=1}^{N}\sigma_x(i)\right]^2 . \tag{1.1}$$

The first two terms represent a Hartree Hamiltonian, and the last term is a residual interaction. The resulting Hamiltonian may be viewed as a generalization of the Lipkin model[1] extended to include a continuous variable. Without the residual interaction, the total azimuthal spin is a good quantum number, and the Hartree states can be classified accordingly. We use the symbol M to denote the expectation of the azimuthal spin operator, $\sum_{i=1}^{N}\sigma_z(i)$. The Hartree Hamiltonian is then given by a shifted oscillator Hamiltonian, and the single particle wave functions are just the oscillator states centered appropriately,

$$\phi_i(z,M,\nu)\sim H_\nu(z+\kappa M)e^{-(1/2)(z+\kappa M)^2} . \tag{1.2}$$

The lowest state for a given M is just the product wave function of ground state oscillator functions at the shifted position. The energy of this state is given by

$$\langle M,\nu_1=0,\nu_2=0,\ldots|H|M,\nu_1=0,\nu_2=0,\ldots\rangle=\frac{N}{2}-\tfrac{1}{2}N\kappa^2M^2 . \tag{1.3}$$

We see that the energy will be lowest for $M=\pm N$, separated by higher energy states for intermediate M. This is just the barrier we are trying to achieve.

The last term in Eq. (1.1) is the residual interaction, which depends on a parameter λ. This term also contains a diagonal interaction, and we will see that the modeling of the tunneling depends on the sign of the coupling.

We note one final simplification in this Hamiltonian. Because the residual interaction depends only on the total spin and the coordinate, $z=\sum_i z_i$, the wave function factorizes into a part depending on z and M and an internal part that does not change. In this work we will only investigate the states of the system which are completely symmetric functions of the coordinates of the various particles. The internal part of the Hamiltonian then plays no role and is henceforth ignored, so the Hamiltonian becomes effectively

$$H'=-\frac{N}{2}\frac{d^2}{dz^2}+\frac{1}{2}\frac{z^2}{N}+\kappa z\left[\sum_{i=1}^{N}\sigma_z(i)\right]+\lambda\left[\sum_{i=1}^{N}\sigma_x(i)\right]^2 . \tag{1.4}$$

The particles in this subspace of states may be treated as bosons.

II. EXACT SOLUTION

We solve the Hamiltonian numerically using as a basis the states of the Hamiltonian without the residual interaction. These states are labeled by the quantum numbers M and ν, the number of quanta of excitation in the shifted harmonic oscillator. The states may be expressed as

$$|M,\nu\rangle=H_\nu[\sqrt{N}(z-\kappa M)]e^{-(1/2)N(z-\kappa M)^2}|M\rangle , \tag{2.1}$$

where $|M\rangle$ is the totally symmetric spin state. The diagonal matrix elements of the Hamiltonian in this basis are

$$\langle M,\nu|H|M,\nu\rangle=\frac{N}{2}+\nu-\tfrac{1}{2}N\kappa^2M^2+\lambda N+\frac{\lambda}{2}(N^2-M^2) . \tag{2.2}$$

The off-diagonal matrix elements connect states M with $M\pm4$, and are given by

$$\langle M-2,\nu|H|M+2,\nu'\rangle=\lambda\left[\left[\frac{N-M}{2}\right]\left[\frac{N+M}{2}\right]\left[\frac{N-M}{2}+1\right]\left[\frac{N+M}{2}-1\right]\right]^{1/2}$$
$$\times e^{-4N\kappa^2}(\nu'!\nu!)^{1/2}\sum_{n=0}^{\min(\nu',\nu)}(-)^{\nu-n}\frac{1}{n!}\frac{1}{(\nu'-n)!}\frac{1}{(\nu-n)!}\left[\left[\frac{N}{2}\right]^{1/2}4\kappa\right]^{\nu'+\nu-2n} . \tag{2.3}$$

Since the Hamiltonian can only flip an even number of spins, the spaces with even and odd numbers of spin are disconnected. Thus in an odd N Hamiltonian the states with $M=\pm N$ are not connected. For simplicity we will only consider even N Hamiltonians and study the states in the space that only include $M=\pm N$. The Hamiltonian is solved by numerical matrix diagonalization. For example, the 40 particle Hamiltonian ($N=40$), truncated to states with $\nu\leq4$, has a dimension of 105.

We now discuss the Hamiltonian parameters appropriate to the nuclear tunneling in spontaneous fission. In a constrained Hartree treatment, the number of level crossings below the barrier is of order 50. We therefore will choose N to have this order of magnitude. This is a large enough number so that the approximation of replacing the discrete index M by a continuous collective coordinate should be permissible.

There are three energy scales in the physical Hamiltonian. The first is the energy of collective single-particle motion. In the fission problem, we identify the single-particle frequency with the giant quadrupole vibration. This has the order of magnitude of 10–15 MeV, and sets the unit scale of the oscillator frequency in Eq. (1.1) or (1.4). The next physical energy scale is the barrier height. For spontaneous fission from the ground state a typical value is 5 MeV. Thus the model Hamiltonian should have a barrier height of about $\frac{1}{2}-\frac{1}{3}$. From Eq. (2.2) we see that both κ and λ can affect the barrier height. It is convenient to define the parameter V_0 which is effectively the barrier height, as we will see in the continuum hopping model,

$$V_0=\tfrac{1}{2}\kappa^2N^3+\frac{\lambda-|\lambda|}{2}N^2 . \tag{2.4}$$

The last physical parameter to be modeled is the strength of the residual interaction that breaks the Hartree symmetry and connects different configurations. The matrix elements between individual Hartree configurations are quite small, but the pairing collectivity builds up the matrix element so that ultimately the pairing gap controls its magnitude. We shall argue elsewhere[2] that for a pairing gap of 1 MeV, the matrix element connecting adjacent configurations (i.e., M to $M\pm4$) has the order of magnitude of 2–3 MeV. Examining Eq. (2.3), we see that the formula for the matrix element depends on M. We shall set the scale of λ by requiring (2.3) to have a magnitude of a few tenths in the middle of the barrier. Unlike κ, the sign of λ is important in the determination of the Hartree solutions. The physical choice is a negative λ, corresponding to an attractive residual interaction. From these considerations, we use the following parameters:

$$N=40,\quad \kappa=0.006\,403,\quad \lambda=-0.0005 . \tag{2.5}$$

For our first exercise we diagonalize the Hamiltonian in a space truncated to $\nu\leq4$. The lower part of the spectrum is shown in Fig. 1. It may be seen that the lowest states are nearly degenerate in pairs, as one ex-

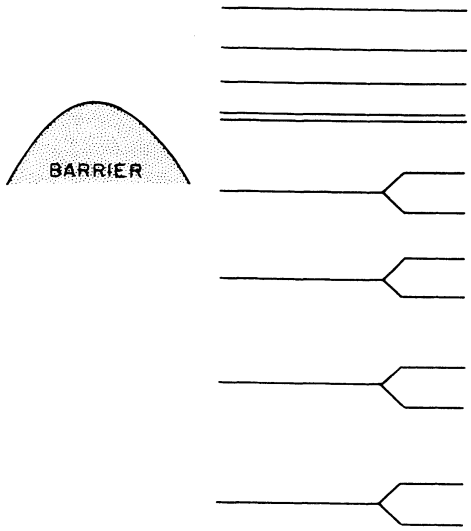

FIG. 1. Spectrum of the Hamiltonian equation (1.1) with the parameter set (2.5). The lowest 10 states are below the potential barrier as defined by Eq. (2.4). These states are nearly degenerate in pairs with the splitting too small to show on the graph for most of the pairs. Only the first three states above the barrier are shown.

pects for a double well Hamiltonian with a barrier in between. The goal of the approximate treatments of the Hamiltonian will be to reproduce the splitting of the degeneracy, as this is the physical characteristic of the barrier penetration. In Table I we record the numerical values of the splittings for this case and also for the truncation to the lowest oscillator state, $\nu=0$. The two spaces give virtually identical splittings (and average energies as well), so the single particle motion is seen to be irrelevant for the tunneling dynamics. Of course, this result depends on the choice of parameters. If the single particle frequency were small compared to the barrier height, the single particle motion might play a role.

III. MEAN-FIELD MODELS

We now discuss various collective treatments of the Hamiltonian based on reducing the Hamiltonian to a one-body Hamiltonian. One can define eigenfunctions of the constrained mean-field Hamiltonian, and use the cranking approximation to treat the dynamics. Or, one can solve the time-dependent mean-field equation in imaginary time to determine the penetrabilities. We shall now apply these methods in turn to the Hamiltonian (1.1).

A. Static mean field solution

In mean-field theory for N symmetric particles, one takes a trial wave function of the form

$$\psi=\prod_{i}^{N}\phi(z_i)\ . \tag{3.1}$$

The mean-field Hamiltonian for the single particle wave function is obtained by taking the expectation value of the Hamiltonian (1.1) and varying ϕ. Since we are interested in the case of large N, we will systematically neglect terms of order $1/N$. The resulting single-particle Hamiltonian, with an external field fz added, is given by

$$H_{\text{s.p.}}=-\frac{1}{2}\frac{d^2}{dz^2}+\tfrac{1}{2}z^2+\kappa\langle\sigma_z\rangle z+\kappa\langle z\rangle\sigma_z$$
$$+2\lambda\langle\sigma_x\rangle\sigma_x+fz\ . \tag{3.2}$$

The external potential is added so that we may constrain the solution to have a continuous range of expectation values $\langle z\rangle$. The single-particle Hamiltonian is seen to have the same z dependence for the upper and lower components of the spin, so the single particle wave function may be expressed as a product of a spin function and a function depending on z. In fact, the z dependence of the Hamiltonian is just a shifted harmonic oscillator, so we may express the single particle wave function as

$$\phi=e^{-(1/2)(z-\langle z\rangle/N)^2}\begin{pmatrix}\cos\left[\frac{\theta}{2}\right]\\ \sin\left[\frac{\theta}{2}\right]\end{pmatrix}\ . \tag{3.3}$$

This Hamiltonian problem is solved by demanding self-consistency for the expectation values of (3.3) in the Hamiltonian (3.2). From the wave function (3.1),(3.3),

TABLE I. Splitting of nearly degenerate pairs of states below the barrier. The logarithm $-\log_{10}(\Delta E)$ is tabulated for each of the approximations described in the text.

Excitation energy	Exact splitting $\upsilon<4$	Exact splitting $\upsilon=0$	Constrained mean field $\langle z\rangle$	Constrained mean field $\langle\sigma_z\rangle$	Continuum	Imaginary time mean field
Ground state	13.0	12.9	19.5	15.3		13.0
0.154	8.96	8.88	14.5	10.0	9.50	8.57
0.289	5.92	5.88	8.3	6.5	6.08	5.39
0.403	3.51	3.52	4.6	3.9	3.55	2.85
0.489	1.92	1.92	2.2	2.1	1.72	1.00

the expectation values of the spin vector (σ_z,σ_x) are

$$\langle\sigma_z\rangle = N\cos\theta, \quad \langle\sigma_x\rangle = N\sin\theta \ . \tag{3.4}$$

This establishes a relation between $\langle\sigma_x\rangle$ and $\langle\sigma_z\rangle$,

$$\langle\sigma_x\rangle = (N^2 - \langle\sigma_z\rangle^2)^{1/2} \ . \tag{3.5}$$

Since (3.3) is a solution to the Hamiltonian (3.2), the orientation of the spin vector is the same as the orientation of the spin field in the Hamiltonian. The spin field is oriented in the direction $(\kappa\langle z\rangle, 2\lambda\langle\sigma_x\rangle)$, and from the proportionality, we infer that either $\langle\sigma_x\rangle = 0$ or, if it is nonzero, $\langle\sigma_z\rangle$ satisfies

$$\langle\sigma_z\rangle = \frac{\kappa\langle z\rangle}{2\lambda} \ . \tag{3.6}$$

These relations are sufficient to express the wave function and the total energy in terms of $\langle z\rangle$.

The solutions to the mean-field equations have several interesting features. First of all, if λ is positive, the lowest solutions have zero expectation of σ_x. As mentioned earlier, λ should be negative on physical grounds, and we only consider that case. Then the mean-field solution may have a nonzero $\langle\sigma_x\rangle$ for a limited range of $\langle z\rangle$. The locus of the expectation values for the constrained solutions for the parameter set (2.5) is graphed in Fig. 2. Near the endpoints of the interval, $\langle\sigma_x\rangle$ is zero and the mean-field state is the pure configuration with $M = \pm N$. Only the z dependence changes in the constrained wave function as it is moved to the point where the locus breaks away from the axis. At that point states of different M mix and the wave function can be continuously deformed from $M = +N$ to $M = -N$.

The mean-field energy in the different regions is given by

$$E_{\text{mean field}} = \begin{cases} \dfrac{N}{2} + \dfrac{\langle z\rangle^2}{2N} - \kappa\,|\langle z\rangle|\,N, & \text{outside barrier} \\ \dfrac{N}{2} + \dfrac{1}{2}\left[\dfrac{1}{N} + \dfrac{\kappa^2}{2\lambda}\right]\langle z\rangle^2 + \lambda N^2, & \text{barrier region} \ . \end{cases} \tag{3.7}$$

These constrained mean-field energies provide the potential energy in a collective Hamiltonian. We now define a collective coordinate x that ranges between -1 and $+1$ as the constrained wave function is moved from one well minimum to the other.

$$x = \frac{\langle z\rangle}{\kappa N^2} \ . \tag{3.8}$$

The collective potential energy is graphed as a function of x in Fig. 3. It may be seen that the different regions are joined smoothly.

We next define the kinetic energy operator in the collective Hamiltonian. It is invariably assumed to have the form

$$K = -\frac{1}{2}\frac{d}{dx}\frac{1}{I}\frac{d}{dx} \ , \tag{3.9}$$

with the inertia I conventionally determined from the cranking formula,[3]

$$I = 2\left\langle \frac{d}{dx}\psi \left| \frac{1}{H_{\text{s.p.}} - E} \right| \frac{d}{dx}\psi \right\rangle \ . \tag{3.10}$$

The inertia derived from this formula may have contributions from the implicit dependence of the mean field spin function on $\langle x\rangle$, as well as the explicit dependence of the spatial wave function in Eq. (3.3). In the outer region the spin wave function does not vary and the inertia is just that of the center of mass motion of N particles

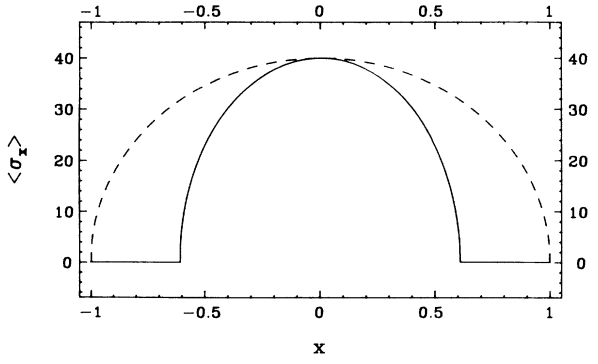

FIG. 2. Collective motion path in constrained mean-field theory. The solid line shows the expectation value of σ_x when the constraining field acts on z. The dashed line shows the same quantities with a constraining field acting on σ_z. The collective variable x is related to $\langle z\rangle$ by Eq. (3.8).

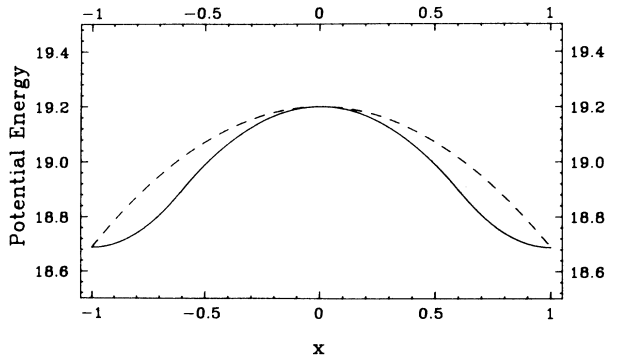

FIG. 3. Collective potential energy in constrained mean-field theory. The solid line is the result for the z constraint, Eq. (3.7), and the dashed line applies to the σ_x constraint, Eq. (3.15).

moving along the z axis,

$$I=2N\left\langle \frac{d}{dx}\phi \middle| \frac{d}{dx}\phi \right\rangle \Big/ (E_{n=1}-E_{n=0})=\kappa^2 N^3 \ . \tag{3.11}$$

To reach the last step, note that the derivative of the oscillator function is $1/\sqrt{2}$ times the first excited state, with an excitation energy of one. The final result would look more familiar if the collective variable were taken as the center-of-mass coordinate, $\langle z \rangle /N$, in which case the derivative would give N for the inertia.

In the barrier region the inertia has an additional term due to the variation of the spin wave function. The derivative operator creates a spin excitation as follows:

$$\frac{d}{dx}\begin{bmatrix} \cos\left[\frac{\theta}{2}\right] \\ \sin\left[\frac{\theta}{2}\right] \end{bmatrix} = \begin{bmatrix} \left[\cos\frac{(\theta+\pi)}{2}\right] \\ \left[\sin\frac{(\theta+\pi)}{2}\right] \end{bmatrix} \times \frac{1}{\left[\frac{4\lambda^2}{\kappa^4 N^2}-x^2\right]^{1/2}}\frac{1}{2} \ . \tag{3.12}$$

The excitation energy of this state is obtained from Eq. (3.2) which yields

$$e_{\theta+\pi}-e_\theta=4\lambda N \ . \tag{3.13}$$

The resulting inertia is given by

$$I=\kappa^2 N^3-\frac{1}{8\lambda N\left[\frac{4\lambda^2}{\kappa^4 N^2}-x^2\right]} \ . \tag{3.14}$$

For the parameters corresponding to the fission problem, the second term in Eq. (3.14) dominates to the extent that the z inertia can be neglected in the barrier region. Of course, it is the entire inertia outside.

One last point that should be mentioned is that the inertia (3.14) becomes singular at the junctions between the barrier and outer regions. This is not fatal, because integrals remain well behaved. In fact the singularity can be transformed away by making a suitable variable transformation.

To investigate this point further, we have also constructed the collective Hamiltonian using $\langle \sigma_z \rangle$ as the constraining field. In that case there is only one domain, and the potential barrier as obtained from the constrained mean-field energy is given by

$$E=\frac{N}{2}-\tfrac{1}{2}\kappa^2 N^3+(\tfrac{1}{2}\kappa^2 N^3+\lambda N^2)(1-x^2) \ . \tag{3.15}$$

The collective path for this constraint is shown in Fig. 2 as the dashed line. The inertia for this Hamiltonian is given by

$$I=\kappa^2 N^3-\frac{1}{8\lambda(1-x^2)} \ . \tag{3.16}$$

We now apply the collective Hamiltonians that we constructed to find the penetrability of the barrier. As mentioned earlier, the physical quantity of interest is the splitting of states of opposite parity with respect to the center of the barrier. However, the energy splitting of eigenstates depends not only on the barrier but on the details of the wave functions in the allowed region. The more degrees of freedom that are active in the allowed region, the smaller will be the amplitude of the wave function at the barrier and the smaller will be the splitting. We therefore need to be careful in comparing the barrier penetration of different models to treat the allowed degrees of freedom on an equal footing. Fortunately, the Wentzel-Kramers-Brillouin (WKB) formula for the splitting of states in a double well separates the dependence on the barrier physics from the dependence on the allowed degrees of freedom. The formula is given by

$$\Delta E=\frac{\omega}{\pi}e^{-\int p\,dx} \ , \tag{3.17}$$

where ω is the classical angular frequency of the motion in the allowed region of the potential.[4] See also the derivation in Refs. 5 and 6. The frequency can also be interpreted as the reciprocal of the derivative of the action for the classically allowed orbit with respect to the energy. This may be related to the energy difference between states in an allowed region as

$$\omega_i=\frac{E_{i+1}-E_i}{2} \ . \tag{3.18}$$

The exponential factor in Eq. (3.17) is the usual WKB integral for the penetration amplitude, with limits of integration at the two classical turning points. In making the comparison with the exact solution, we shall apply Eqs. (3.17) and (3.18) taking the density of states from the actual Hamiltonian. We will then be insensitive to any shortcomings of the collective model in the allowed region.

The results for the splitting are shown in Table I, in columns 4 and 5. To get a ground state splitting, we extrapolated the level density, Eq. (3.18). We see that the $\langle z \rangle$-constrained mean-field approximation works reasonably well for states not too far from the barrier top, but is poor for states far below the barrier. By comparison, the $\langle \sigma_z \rangle$-constrained theory is much better for the low states. This shows that the constrained Hartree theory is very dependent on the choice of path, and that an *a priori* guess at the appropriate path might be quite misleading.

Physically, we know that the dynamics in the barrier are governed by changing the spin occupation, which corresponds to level crossings of single-particle states of different nodal structure in the physical problem. Hence it is reasonable that constraining the spin occupation directly gives a better approximation than influencing it only indirectly through constraining the collective variable z. Note that the usual practice in constrained Hartree-Fock calculations corresponds to the latter: constraining the deformation and hoping that this will indirectly influence the change in orbital occupation.

B. Imaginary time mean field theory

A new method for treating collective tunneling in many-particle physics was proposed by Levit *et al.*,[6] following a technique originally introduced for bubble formation[7] and applied extensively in field theory.[8] The method is based on a functional integral representation of the resolvent of the many-particle Hamiltonian. The result of the theory, applied to the double-well Hamiltonian, is an energy splitting which has the same appearance as Eq. (3.14). It is given by[6]

$$\Delta E = \frac{\omega}{\pi} e^{-P} . \tag{3.19}$$

Here ω is the frequency of motion in either of the wells, and P is a penetration integral given by

$$P = \frac{N}{2} \int_{-T/2}^{T/2} dt \langle \phi(-t) | \partial_t | \phi(t) \rangle . \tag{3.20}$$

The wave function ϕ is determined from the imaginary time mean-field equation,

$$\partial_t \phi(z,t) + \left[-\frac{\partial^2}{2\partial z^2} + \frac{z^2}{2} + \kappa \langle \sigma_z \rangle_t z + \kappa \langle z \rangle_t \sigma_z + 2\lambda \langle \sigma_x \rangle_t \right] \phi(z,t) = \epsilon \phi(z,t) . \tag{3.21}$$

The expectation values in the imaginary time equations are evaluated replacing $\phi^*(t)$ by $\phi(-t)$; for example,

$$\langle \sigma_z \rangle_t = \langle \phi(-t) | \sigma_z | \phi(t) \rangle , \tag{3.22}$$

and similarly for other operators. The solutions are required to satisfy the boundary condition,

$$\phi\left[-\frac{T}{2}\right] = \phi\left[\frac{T}{2}\right] . \tag{3.23}$$

The boundary $\phi(\pm T/2)$ should match an allowed region solution at the edge of the barrier. We only know how to impose the periodicity and this matching condition for the ground state tunneling, in which case the boundary ϕ is the ground state mean-field solution in an allowed region. The wave function ϕ becomes identical to the allowed solution on the other side of the barrier at $t=0$. It passes through the barrier at finite $|t|$ between 0 and $|T/2|$.

The imaginary time equations are solved following the method of Ref. 9. We start from a wave function representing a small-amplitude oscillation about the saddle point of the barrier. The wave function is iteratively modified to extend it to large amplitudes, and the limits of T are simultaneously increased. In principle, the limits on T should be extended to infinity, but large T does not contribute the ground state penetration and the limits can be left at some large finite value.

Some properties of the wave function for the parameter set (2.5) are shown in Figs. 4–6. The expectation value of z is displayed as a function of t in Fig. 4. At large negative time, $\langle z \rangle$ approaches asymptotically the value $-\kappa N$, which is the expectation in the ground state of the left-hand well. As t varies from $-T/2$ to 0, the wave packet moves through the barrier and approaches the ground state of the right-hand well at $t=0$. The wave function itself does not change shape as it moves through the barrier, as is to be expected for a harmonic oscillator Hamiltonian perturbed by a linear potential.

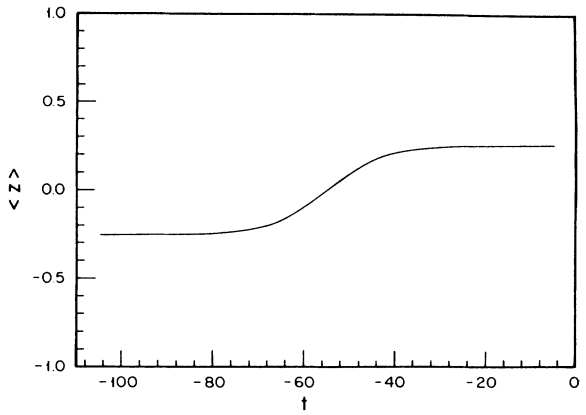

FIG. 4. Time dependence of $\langle z \rangle$ in imaginary time mean-field theory. Only negative values of time are shown; $\langle z \rangle_t = \langle z \rangle_{-t}$.

The relation between $\langle \sigma_z \rangle$ and $\langle z \rangle$ is shown in Fig. 5. It is very close to linear. This tells us that the optimal path connecting the two wells moves evenly in the two coordinates. By contrast, the $\langle z \rangle$-constrained mean-field solution behaved quite abruptly, with $\langle \sigma_z \rangle$ constant for part of the trajectory. In Fig. 5 we display $\langle \sigma_x \rangle$ as a function of the position x, defined in terms of $\langle z \rangle$ by Eq. (3.8). Qualitatively the behavior is very similar to the $\langle \sigma_z \rangle$-constrained mean field. However, the relation (3.5) is no longer satisfied, because the imaginary time wave functions are not normalized in the usual way. In fact, with the imaginary time wave function the σ_y operator has a nonvanishing expectation value. It is imaginary, corresponding to an imaginary momentum for a particle tunneling under a barrier.

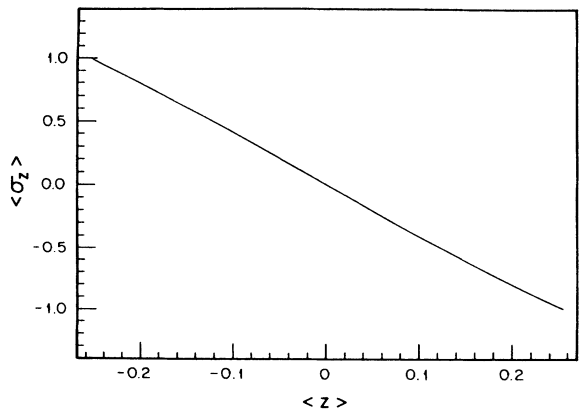

FIG. 5. Relation between $\langle \sigma_z \rangle$ and $\langle z \rangle$ in imaginary time mean-field theory, as t varies from -100 to 0.

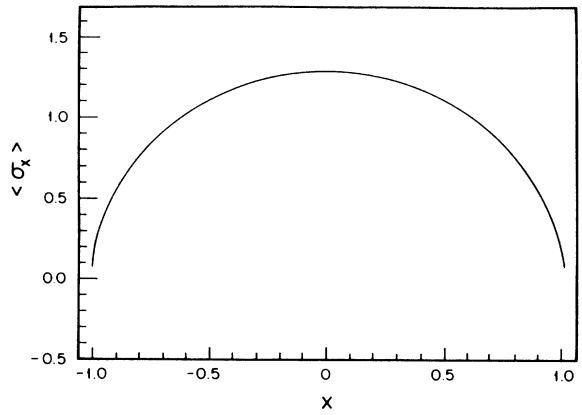

FIG. 6. Variation of $\langle \sigma_x \rangle$ in imaginary time mean-field theory, as t varies from -100 to 0. To facilitate comparison with the constrained mean-field behavior, Fig. 2, this has been plotted as a function of x defined in terms of $\langle x \rangle$ by Eq. (3.8). Note that in the barrier region $\langle \sigma_x \rangle$ exceeds N, its maximum value in real time wave functions.

Whereas the penetrability is well defined and straightforwardly calculable for any energy, the premultiplying factor in Eq. (3.19) is more difficult. For the ground state, it is unambiguously defined as the ratio of two determinants in the dilute instanton gas approximation.[8] This is normally approximated by the collective frequency ω in the outer well. In our case this is the harmonic oscillator frequency $\omega=1$. We also used this prescription for calculating the splitting of excited states, although in that case the formula cannot be derived by matching solutions in the inner and outer regions. As the energy is increased, it is clear physically that other degrees of freedom play increasingly important roles, so this prescription will systematically overestimate the splitting.

The results of the imaginary time calculation of ground-state energy splittings are shown in Table II for a range of parameters in the Hamiltonian. The parameters were varied keeping the barrier height the same. We see that there is impressive agreement between the numerical splittings and the results of the imaginary time method. In the present case, one can understand the accuracy of the stationary-phase approximation by noting that the functional integral for our model Hamiltonian may be rescaled as in Eq. (6.15) of Ref. 5 to have an explicit factor of N in the exponent, so that the present result is the first term in an asymptotic $1/N$ expansion with $N=40$. Results for excited states are shown in the last column of Table I. As expected, the errors introduced by the premultiplying factor increase with increasing energy.

TABLE II. Ground state energy splittings. The exact numerical values of $-\log_{10}(\Delta E)$ for a variety of parameter sets are compared with the imaginary time results, Eqs. (3.16)–(3.20).

Parameters		Splitting	
λ	κ	Exact	Eq. (3.16)
−0.0004	0.006	14.21	14.25
−0.0005	0.006 403	12.96	13.02
−0.0006	0.006 782	12.00	11.96
−0.0007	0.007 1413	11.22	11.21

IV. CONTINUUM HOPPING MODEL

In this section we discuss a collective model based on the structure of the Hamiltonian as a band diagonal matrix.[2] As we have seen, the configuration space can be truncated to $\nu=0$ with no loss of accuracy in the parameter range relevant for nuclear problems. Then the Hamiltonian matrix is tridiagonal, and it can be approximated by a Hamiltonian in a continuum coordinate in just the same way that continuous Hamiltonians are approximated by matrices on a discrete mesh. If adjacent elements represent steps of a continuous coordinate by an amount Δx, then the Hermitian tridiagonal matrix

$$\begin{bmatrix} E_1 & v_1 & 0 & \cdots \\ v_1 & E_2 & v_2 & \cdots \\ 0 & v_2 & E_3 & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{bmatrix} \tag{4.1}$$

is represented by the continuous operator

$$H_{\rm coll} = -\frac{d}{dx}\Delta x^2 v(x)\frac{d}{dx} + E(x) + 2v(x) \ . \tag{4.2}$$

We apply this to the Hamiltonian equations (2.2) and (2.3), and find for the collective Hamiltonian the following,

$$H_{\rm coll} = -4\,|\,\lambda\,|\,\frac{d}{dx}(1-x^2)\frac{d}{dx} + V_0(1-x^2) + \frac{N}{2} - \frac{\kappa^2 N^3}{2} + (\lambda - |\,\lambda\,|)N \ , \tag{4.3}$$

where V_0 is defined in Eq. (2.4). Note that this collective model can be formulated for either sign of the interaction parameter λ, unlike the constrained Hartree models. In the case of repulsive λ, the phase of the wave function is redefined to produce positive relative phases for the ground state wave function. This is the origin of the absolute values in Eq. (4.3). In keeping with the continuum limit, we have also dropped terms of order $1/N$ in the kinetic operator.

The Hamiltonian (4.3) has a simple enough algebraic structure for its penetrability integral to be expressible in terms of standard mathematical functions. The integral is given by

$$\int p\,dx = \left[\frac{V_0}{|\,\lambda\,|}\right]^{1/2} \int \left[\frac{x_t^2 - x^2}{1-x^2}\right]^{1/2} dx = \left[\frac{V_0}{|\,\lambda\,|}\right]^{1/2} [E(x_t^2) - (1-x_t^2)K(x_t^2)] \ , \tag{4.4}$$

where the elliptic functions $E(y)$ and $K(y)$ are defined in

Ref. 10. The results of this model are shown in the last column of Table I. We see that the model is fairly accurate for energies not too far below the barrier.

The continuum limit can only be a good approximation if the change in the wave function amplitude is small going from one state to the next. This breaks down very far below the barrier, and so we expect the model to become inaccurate there.

Comparing the continuum model with Eqs. (3.12) and (3.13), we see that it is very similar to the cranked $\langle \sigma_z \rangle$ collective Hamiltonian. The only difference is an additional term in the cranked inertia, associated with the particle motion in the z coordinate. For the parameter range of nuclear interest, that term is negligible in the Hamiltonian.

V. CONCLUSION

The physics of the Hamiltonian (1.1) has been shown to be rich enough to test and compare the major treatments of large scale collective motion. The comparision is very illuminating, exhibiting behavior that up to now has been discussed in a much more abstract way.

From the constrained Hartree calculations, we find that the barrier penetration can be quite dependent on the choice of constraint, which affects the collective path the system takes to traverse the barrier. This vindicates the claim made by advocates of the imaginary time mean-field treatment, that one should not make an *a priori* choice of path but rather use a theory that selects the optimal path for the process under consideration.

Another thing that became very clear is that different schemes supplement each other in having different domains of validity. The continuum hopping model was seen to be quite powerful, but limited to excited states for two reasons. Since it only treats well the barrier penetration aspect, it should be used at a high enough excitation so that the nonbarrier degrees of freedom can be separated out via the level density factor. Also, the approximation intrinsically breaks down at very negative energies. By contrast, the imaginary time mean-field theory has no obvious limitations concerning barrier height, but ambiguity in the premultiplying factor presently limits its applicability to ground states.

One aspect of the physics that was not so clear beforehand, which this study helps illuminate, is the role of the single particle motion in the barrier penetration. The accuracy of the $\nu=0$ truncation shows that the single particle motion, participating for example by the virtual excitation of giant quadrupole amplitudes, can be ignored. This conclusion is also known from studies of the cranked Hartree-Bogoliubov model;[11] the pairing contribution to the inertia completely dominates the single-particle contribution. This is seen in our cranked σ_z mean-field model, which has two terms in the inertia. The interaction term is completely dominant for parameter ranges of interest in the spontaneous fission problem. The $\nu=0$ truncation allows a model to be applied in which the inertia is identical to the second term of this cranked expression. Out of curiousity we increased the parameter κ to make the two terms comparable. Then the $\nu=0$ truncation overpredicts the penetrability substantially, showing that the single-particle term can increase the inertia in a suitable parameter domain.

One of our original goals in this study was to gain insight into what actually breaks the Hartree symmetry—is it the pairing interaction or is it the density-density interaction that is amenable to the imaginary time mean-field approach? On a physical Hamiltonian level, there is not much to distinguish these mechanisms; a local contact interaction of strength 300 MeV fm^3 is adequate to generate realistic pairing as well as to provide a fluctuating mean field of reasonable strength. Since both the continuum hopping treatment and the imaginary mean-field method work well in their domains, as far as our model goes the two treatments are not incompatible. However, there is one aspect of the physical pairing dynamics that would seem to be difficult to reproduce with mean-field treatments, namely odd-even effects in penetration factors. Unfortunately, our model is not sufficiently realistic to exhibit this feature of the dynamics, and so this question is not yet resolved.

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