Nuclear fission with mean-field instantons

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We present a description of nuclear spontaneous fission, and generally of quantum tunneling, in terms of instantons, that is, periodic imaginary-time solutions to time-dependent mean-field equations. This description allows comparisons to be made with the more familiar generator coordinate (GCM) and adiabatic time-dependent Hartree-Fock (ATDHF) methods. It is shown that the action functional whose value for the instanton is the quasiclassical estimate of the decay exponent fulfills the minimum principle when additional constraints are imposed on trial fission paths. In analogy with mechanics, these are conditions of energy conservation and the velocity-momentum relations. In the adiabatic limit, the instanton method reduces to the time-odd ATDHF equation, with collective mass including the time-odd Thouless-Valatin term, while the GCM mass completely ignores velocity-momentum relations. This implies that GCM inertia generally overestimates the instanton-related decay rate. The very existence of the minimum principle offers hope for a variational search for instantons. After the inclusion of pairing, the instanton equations and the variational principle can be expressed in terms of the imaginary-time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory. The adiabatic limit of this theory reproduces ATDHFB inertia.

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I. INTRODUCTION

Decay of a metastable state of a system of interacting fermions or bosons is an important phenomenon relevant to nuclear, atomic, and condensed matter physics. The calculation of decay rate requires the exact knowledge of the wave function in the proper asymptotic region, which is usually very difficult to achieve for many-body systems. In fact, very often the only feasible description of systems including hundreds or more particles relies on the quantum mean-field theory. Unfortunately, such theory does not contain quantum tunneling. This gives rise to a notorious arbitrariness in calculations of decay rates or half-lives which concerns a selection of relevant degrees of freedom and prescriptions for potential and inertia parameters.

Specifically, within the Hartree-Fock (HF) method, static equations give only saddle points of energy,

$$\mathcal{H}[\psi^*, \psi] = \int dx \sum_k \frac{\hbar^2}{2m} \nabla\psi_k^* \nabla\psi_k + \mathcal{V}[\psi^*, \psi], \qquad (1)$$

with $\mathcal{V}[\psi^*, \psi]$ being potential energy, so one has to resort to the time-dependent HF (TDHF) equations for dynamics

$$i\hbar\partial_t \psi_k(t) = \hat{h}(t)\psi_k(t) = -\frac{\hbar^2}{2m}\nabla^2\psi_k(t) + \frac{\delta\mathcal{V}}{\delta\psi_k^*(t)}, \qquad (2)$$

with the mean-field single-particle (s.p.) Hamiltonian $\hat{h}(t)$ given by $\hat{h}[\psi^*(t), \psi(t)]\psi_k(t) = \delta\mathcal{H}/\delta\psi_k^*(t)$, and the self-consistent s.p. potential $\hat{V}(t)$ given by $\delta\mathcal{V}/\delta\psi_k^*(t) = \hat{V}(t)\psi_k(t)$. For the case of energy $\mathcal{H}$ given by a density functional, we assume in the following (if not indicated otherwise) that it has properties of the expectation value of the Hamiltonian. Although Eqs. (2) looks like the Schrödinger equation, in fact, it is a classical field equation as a result of the nonlinear dependence of $\hat{h}$ on ψ_k. The energy of Eq. (1) and the overlaps $\langle\psi_k \mid \psi_l\rangle$ are conserved by Eqs. (2). The energy conservation forbids a tunneling within TDHF, i.e., an escape from a minimum of $\mathcal{H}$ with energy lower than the saddle. Evidently, this comes about by projection of the full many-body theory onto Slater states.

A quasiclassical treatment of quantum tunneling within the many-body mean-field theory, which is a natural generalization of the Gamow treatment of α decay to an infinite-dimensional system of fields, leads to instantons, i.e. imaginary-time solutions to TDHF equations [1]. This method exploits an idea of trajectories evolving in imaginary time [2] which emerge from the stationary-phase approximation to the path-integral expression for $\mathrm{Tr}(E - \hat{H})^{-1}$. The decay rate of a metastable state is proportional to $\exp(-S/\hbar)$, where S is action for the optimal instanton. We do not consider here a prefactor coming from quantum fluctuations around the optimal path.

For a particle in an external potential, such an optimal decay trajectory describes classical motion in the inverted potential. It starts at the metastable state (being a local maximum of the inverted well) and returns there after bouncing from the inverted barrier, hence the name "bounce." For a system of interacting fermions, one has to transform TDHF Eqs. (2) to imaginary time, i.e., formally, $t \to -i\tau$. Under this transformation, $\psi \to \psi(x, -i\tau) = \phi(x, \tau)$ and $\psi^* \to \psi(x, -i\tau)^* = \phi(x, -\tau)^*$ [1, 3]. It follows that density $\rho(x, t) = \psi^*(x, t)\psi(x, t)$ transforms to $\rho(x, \tau) = \phi(x, -\tau)^*\phi(x, \tau)$. This has important consequences. First, the mean-field equations in imaginary time [1,3,4]

$$\hbar\frac{\partial\phi_k}{\partial\tau}(\tau) = -(\hat{h}(\tau) - \epsilon_k)\phi_k(\tau) = \frac{\hbar^2}{2m}\nabla^2\phi_k(\tau) - \frac{\delta\mathcal{V}}{\delta\phi_k^*(-\tau)} + \epsilon_k\phi_k(\tau), \qquad (3)$$

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are nonlocal in τ, as $\mathcal{V}$ as well as $\hat{h}(\tau) = \hat{h}[\phi^*(-\tau), \phi(\tau)]$ depend on both $\phi(x,\tau)$ and $\phi(x,-\tau)$. Second, density $\rho(x,\tau)$, generally complex or piecewise negative, does not correspond to any Slater determinant, unlike in the real-time dynamics. In analogy with TDHF, Eqs. (3) conserve energy $\mathcal{H}(\tau) = \mathcal{H}[\phi^*(-\tau), \phi(\tau)]$, with

$$\mathcal{H}(\tau) = \int dx \sum_k \frac{\hbar^2}{2m} \nabla\phi_k^*(-\tau)\nabla\phi_k(\tau) + \mathcal{V}[\phi^*(-\tau), \phi(\tau)]. \tag{4}$$

The above formula means that one obtains $\mathcal{H}(\tau)$ replacing everywhere $\psi_k^*(t)$ by $\phi_k^*(-\tau)$ in the usual form of the energy functional. Since the Hamiltonian is Hermitian, i.e., $\hat{H}^+ = \hat{H}$, it follows that $\mathcal{H}(-\tau) = \mathcal{H}^*(\tau)$, and the mean-field Hamiltonian $\hat{h}(\tau)$, defined by $\hat{h}(\tau)\phi(\tau) = \delta\mathcal{H}/\delta\phi^*(-\tau)$, fulfills the condition $\hat{h}(-\tau) = \hat{h}^+(\tau)$. The latter ensures that Eqs. (3) *without the $\epsilon_k\phi_k$ term* conserves the overlaps: $\frac{d}{d\tau}\langle\phi_i(-\tau) \mid \phi_j(\tau)\rangle = 0$. The complete Eqs. (3) still conserves diagonal overlaps, while giving the exponential time dependence to the off-diagonal ones. However, those overlaps remain zero for all τ, if they equal zero at some τ. As usual, the saddle point approximation to the path integral leads to the periodicity condition for the optimal trajectories. Hence, bounce is a periodic instanton,

$$\phi_k(T/2) = \phi_k(-T/2), \tag{5}$$

and the periodicity is enforced by the $\epsilon_k\phi_k$ term in Eqs. (3). The physical context imposes the specific boundary conditions on bounce. For a description of the decay of a metastable ground state, the initial (and thus also the final) states have to be chosen equal to the HF solutions ψ_k^{HF} at the metastable minimum, $\phi_k(T/2) = \phi_k(-T/2) = \psi_k^{\mathrm{HF}}$, with total energy E_{gs}, and the parameters ϵ_k must be equal to the HF s.p. energies at this minimum. The s.p. states $\phi_k(\tau = 0)$ form some normal [as $\phi_k^*(-\tau) = \phi_k^*(\tau)$ at $\tau = 0$] HF state at energy $\mathcal{H} = E_{\mathrm{gs}}$ on "the other side of the barrier." The periodicity condition together with the initial condition fix the particular constant values of the overlaps as

$$\langle\phi_i(-\tau) \mid \phi_j(\tau)\rangle = \delta_{ij}. \tag{6}$$

The decay exponent is given by [1,3]

$$S = \hbar \int_{-T/2}^{T/2} d\tau \sum_k \left\langle \phi_k(-\tau) \middle| \frac{\partial\phi_k}{\partial\tau}(\tau) \right\rangle. \tag{7}$$

Bounce penetrates the static barrier, which is impermeable for real-time solutions at the same energy, practically in a finite time interval around $\tau = 0$ and becomes infinitely slow close to the endpoints, so that T extends to infinity [1,3,4]. Equations (3) determine both decay channels and decay probabilities. No additional assumptions are necessary, as they form a complete quasiclassical solution to the tunneling problem within the mean-field theory.

Up to now, solutions of Eqs. (3) have been obtained only for relatively simple systems [1,3–7]. The task of finding instantons seems rather hopeless without a special treatment: to handle nonlocality in τ, one could try to solve Eqs. (3) together with

$$-\hbar\frac{\partial[\phi_k(-\tau)]}{\partial\tau} + (\hat{h}(-\tau) - \epsilon_k)\phi_k(-\tau) = 0, \tag{8}$$

describing instantons evolving backward, obtained from Eqs. (3) by using the identity $(\partial_\tau f)(-\tau) = -\partial_\tau(f(-\tau))$. However, Eq. (8) describes the inverse diffusion [cf. signs of time and spatial derivatives in Eqs. (3) and (8)], which leaves no hope for a stable solution. The problem seems more difficult than a search for periodic solutions of the real-time TDHF equations, which is known to be difficult enough. In the presented form, the instanton approach did not lead to any comparisons with the existing studies of fission, which are mostly based either on the generator coordinate method (GCM) in the Gaussian overlap approximation (GOA) or on the adiabatic TDHF (ATDHF) method, either in its extreme cranking or some more refined version.

In this work, we present the instanton method in familiar terms of the HF or HFB theory. This helps one to grasp the similarities and differences between this and other methods and to clarify their interrelations. In particular, the instanton turns out to be an imaginary-time analog of the self-consistent TDHF solution in the representation of the time-even and time-odd components of the density matrix [8]. Both produce the same inertia in the ATDHF limit, when one includes time-odd components only to the first order.

Moreover, it turns out that instanton action in Eq. (7) is the minimum value of the action functional over a properly constrained set of trial fission trajectories defined in the space of Slater determinants [9]. Thus, any fission path that satisfies these constraints provides the upper bound for the decay exponent. This offers hope for a variational approach to finding instantons. One may also expect that a good estimate of action may be easier to find than that of the instanton itself.

The starting point is the realization that Eqs. (3) describe two different sets of Slater determinants, bra $\Phi(-\tau)$ built out of $\phi_k(-\tau)$, and ket $\Phi(\tau)$ built out of $\phi_k(\tau)$, while energy $\mathcal{H}$ is equal to the off-diagonal energy overlap kernel in the sense of GCM, that is, $\langle\Phi(-\tau)|\hat{H}|\Phi(\tau)\rangle/\langle\Phi(-\tau)|\Phi(\tau)\rangle$ [9]. It is the difference between bra and ket that makes barrier tunneling possible and allows the conservation of energy [Eq. (4)]. The energy overlap kernel reduces to $\langle\Phi(-\tau)|\hat{H}|\Phi(\tau)\rangle$ owing to the choice of the overlap value $\langle\Phi(-\tau)|\Phi(\tau)\rangle = 1$ that follows from $\langle\phi_k(-\tau)|\phi_l(\tau)\rangle = \delta_{kl}$. However, the overlap of the normalized bra and ket, $(\langle\Phi(-\tau)|\Phi(-\tau)\rangle\langle\Phi(\tau)|\Phi(\tau)\rangle)^{-1/2}$, is smaller than 1. Bounce may be thought of as one of many trial tunneling paths $\{\phi_k\}$, each given as two sets of wave functions, $\{\phi_{1k}(\tau)\}$ and $\{\phi_{2k}(\tau)\}$, defined on the interval $[0, T/2]$, and related to the variables of Eqs. (3):

$$\phi_k(\tau) = \begin{Bmatrix} \phi_{1k}(-\tau) & \text{for } \tau < 0, \\ \phi_{2k}(\tau) & \text{for } \tau > 0 \end{Bmatrix}. \tag{9}$$

At $\tau = 0$, both Φ_1 and Φ_2 are equal to some constrained HF (CHF) state $\Phi(0)$ at the outer slope of the barrier with the constraint $-\partial_\tau\Phi(0)$. Equations (3) and (8), rewritten in terms of $\phi_{1k}(\tau)$ and $\phi_{2k}(\tau)$, are

$$\hbar\partial_\tau\phi_{2k} + (\hat{h}(\tau) - \epsilon_k)\phi_{2k} = 0,$$
$$-\hbar\partial_\tau\phi_{1k} + (\hat{h}^+(\tau) - \epsilon_k)\phi_{1k} = 0, \quad (10)$$

with $\hat{h}(\tau) = \hat{h}[\phi_{1k}, \phi_{2k}]$. It should be clear that one can equally well use fields restricted to $[-T/2, 0]$.

The paper is organized as follows: The main results for the HF instanton method are contained in Secs. IV–VII. These are the variational principle (Sec. IV), the formulation in terms of coordinates and momenta and comparison with the cranking method (Sec. V), the introduction of special variables in the form of the time-even density matrix and the time-odd Hermitian operator that make plain the adiabatic limit of the theory (Sec. VI), and the demonstration that the GCM+GOA action follows from that for instanton after neglecting the velocity-momentum relations (Sec. VII). In Sec. VIII, these results are generalized to systems with pairing. Section III prepares useful formulas for later sections. Section II introduces some unusual features of the instanton method. Conclusions are given in Sec. IX.

II. GENERAL OVERVIEW

A few comments on several unusual features of the instanton equations may be helpful. As the linear combination of the s.p. wave functions changes their Slater determinant only up to a factor, one may expect that the instanton equations may be more general than Eqs. (3), which fixes in a specific way the lengths and angles among each of the sets $\{\phi_{1k}\}$ and $\{\phi_{2k}\}$ separately. Such a more general equation will imply a more general expression for the instanton action than Eq. (7), and both will be given in the next section.

The nonlocal in time form of the instanton equations follows directly from the transformation of the standard variational principle of the TDHF theory, $\delta\int\langle\Psi(t)|i\hbar\partial_t - \hat{H}|\Psi(t)\rangle dt = 0$, to imaginary time, $\delta\int\langle\Phi(-\tau)|\hbar\partial_\tau + \hat{H}|\Phi(\tau)\rangle d\tau = 0$. Equations (3) and (8), without the periodicity-fixing terms, have the canonical form in strange variables

$$\hbar\frac{\partial\phi_k(\tau)}{\partial\tau} = -\frac{\delta\mathcal{H}}{\delta\phi_k^*(-\tau)},$$
$$\hbar\frac{\partial[\phi_k^*(-\tau)]}{\partial\tau} = \frac{\delta\mathcal{H}}{\delta\phi_k(\tau)}, \quad (11)$$

none of which has a determined time parity. The usual canonical variables are τ-even coordinates and τ-odd momenta. Such standard coordinates and momenta may be introduced by a change of variables with the resulting equations of motion local in time and canonical in form (Sec. V). It should be stressed that a local form of the instanton equations does not facilitate their solution but makes easier their comparison to other theories of the large amplitude collective motion (LACM). One possibility is given [3] by $\phi_k = \sqrt{\rho_k}\exp(-\chi_k)$, with ρ_k time-even and χ_k time-odd. For one real-valued wave function and potential energy being a functional of density, $\mathcal{V}[\rho]$, one obtains the continuity and "fluid velocity" equations, as for the density-phase representation of the Schrödinger equation. Energy $\mathcal{H}$ becomes

$$\mathcal{H} = \frac{\hbar^2}{m}\int dx\left[-\frac{\rho(\nabla\chi)^2}{2} + \frac{(\nabla\rho)^2}{8\rho}\right] + \mathcal{V}[\rho], \quad (12)$$

where the minus sign shows the role of χ in the lowering of energy down to E_{gs} in the barrier region. From the boundary conditions, symmetries of ρ and χ, and the continuity equation, one obtains action $S = (\hbar^2/m)\int d\tau dx \rho(\nabla\chi)^2$. For simple systems, such as the Bose-Einstein condensate of ^{7}Li atoms, this framework allows the exact treatment of the collapse of the metastable state [7]. However, the density-phase variables seem unsuitable for fermions because of the spinor structure and the rearrangement of nodes of s.p. wave functions along the barrier that makes phases singular. More appropriate variables are defined in Secs. V and VI.

The other peculiarity of Eqs. (3) is that it may be thought of as describing a forced motion. The mean field $\hat{h}$ that causes the evolution of $\Phi(\tau)$ depends on $\Phi(-\tau)$, so one may say that one state drags the other. More specifically, as climbing the barrier is impossible without an external drive, the drag is necessary at the beginning of the motion from the metastable state through the barrier and at the beginning of the return motion to the metastable minimum. Action Eq. (7) is given by the integral of the scalar product between the change in the driven state and the state that drives it. For motions for which the result of the dragging is fixed by the instanton boundary conditions, there must be some minimal dragging that causes this (fixed) result. Hence, one can expect that there is a minimum principle that selects instantons. If so, then solving Eqs. (3) and finding the decay exponent could be done by a minimization of a functional. The functional is practically given by Eq. (7). What remains to be done is to learn the necessary additional constraints that make this action minimal for instantons.

In fission studies, mean-field states are parametrized by expectation values of observables that provide coordinates along the barrier, called deformations. Consider as an example the quadrupole moment $\hat{Q}$. For bounce states $\Phi(\tau)$, one has two possible labels. Within the imaginary-time formalism, a natural choice is $Q(\tau) = \langle\Phi(-\tau)|\hat{Q}|\Phi(\tau)\rangle = \sum_k\langle\phi_k(-\tau)|\hat{Q}|\phi_k(\tau)\rangle$. Since $\hat{Q}$ is Hermitian, $Q(-\tau) = Q^*(\tau)$, and $\dot{Q}(\tau) = dQ/d\tau = \sum_k\langle\phi_k(-\tau)|[\hat{h}(\tau), \hat{Q}]|\phi_k(\tau)\rangle$, with $\dot{Q}(-\tau) = -\dot{Q}^*(\tau)$. Thus the real part of $\dot{Q}(\tau)$ fixes $\tau = 0$ as the return (or bounce) point. Another possibility is to trace the deformation of the normalized state $\Phi(\tau)$, that is, $q(\tau) = \langle\Phi(\tau)|\hat{Q}|\Phi(\tau)\rangle/|\Phi(\tau)|^2$. Generally, $q(\tau) \neq Q(\tau)$ and $q(\tau) \neq q(-\tau)$, except for $\tau = 0$ and $\pm T/2$.

Instanton cannot depend solely on a time-even variable like the real part of Q, as then Eqs. (3) at $\tau = 0$ would require a static HF solution without constraints which cannot exist on the barrier slope. One can observe that the derivative $\dot{q}(\tau = 0)$ is equal to $2\Re\sum_k\langle[\partial_\tau\phi_k(0)]_\perp|\hat{Q}|\phi_k(0)\rangle$, where $[\partial_\tau\phi_k(0)]_\perp$ is perpendicular to all $\phi_k(0)$. Considering $\Phi(0)$ as a stationary HF state with the constraint $-\partial_\tau\Phi(0)$, one can see that $\dot{q}(0)$, up to a positive constant, is the scalar product of two constraints: the one of instanton at $\tau = 0$ [Eqs. (3)] and the other, $-\hat{Q}\Phi(0)$, the proper quadrupole constraint on the slope where $\partial\mathcal{H}/\partial Q < 0$. Since $\phi_k(0)$ lives on this slope and has the quadrupole moment $Q(0)$, it must be close to some $\hat{Q}$-constrained HF state. Hence this scalar product and the derivative $\dot{q}(0)$ are very likely positive. Indeed, it was found positive in the simple model [7]. If so, the return point for the coordinate $q(\tau)$ is at $\tau > 0$, which means that at $\tau = 0$ the quadrupole moment of the normalized state Φ_2 still increases, while that of Φ_1 (instanton evolving backward) decreases. Moreover, as calculations show for simple systems, states ϕ_{1k} and ϕ_{2k} with the same q are different. Thus, neither Q nor q are sufficient as labels for bounce.

In general, the instanton mean field is not Hermitian. The condition it satisfies, $\hat{h}(-\tau) = \hat{h}^+(\tau)$, imposes the following conditions on the Hermitian and anti-Hermitian parts of its standard decomposition: $\hat{h}(\tau) = \hat{h}_R(\tau) + \hat{h}_A(\tau)$, $\hat{h}_R(-\tau) = \hat{h}_R(\tau) = \hat{h}_R^+(\tau)$, and $\hat{h}_A(-\tau) = -\hat{h}_A(\tau) = \hat{h}_A^+(\tau)$. The anti-Hermitian mean field $\hat{h}_A$ comes from τ-odd components of densities appearing in energy $\mathcal{H}$, either in the form of the expectation value of $\hat{H}$ or in the form of the energy functional. In the latter case, as for the Skyrme energy functional, the generic contribution to $\hat{h}_A$ in the tunneling problem comes from the current density $\mathbf{j}$. In the imaginary-time formalism, it takes a form $\mathbf{j}(\tau) = \sum_k [\phi_k(\tau)\nabla\phi_k^*(-\tau) - \phi_k^*(-\tau)\nabla\phi_k(\tau)]/2$, which follows from this part of Eqs. (3) that shows the continuity of the probability flow. It follows that $\mathbf{j}(-\tau) = -\mathbf{j}^*(\tau)$. This differs by the factor $(-i)$ from the conventional current in the real-time TDHF. As a result, the time-odd contribution to the TDHF mean field $i \cdot \mathbf{j} \cdot \nabla$ becomes $-\mathbf{j} \cdot \nabla$ in the imaginary-time formalism. Its anti-Hermitian part is proportional to *the real part* of $\mathbf{j}(\tau)$, and the latter appears as soon as the real parts of functions $\phi_k(\tau)$ and $\phi_k(-\tau)$ become different. The time-odd mean field $\hat{h}_A$ is the immediate imaginary-time analog of the Thouless-Valatin potential in TDHF [10], and we will use this name for it.

III. VARIOUS FORMS OF INSTANTON ACTION AND EQUATIONS

The value of S that determines the fission probability relies only on a part of the information contained in the bounce solution. By using the general identities $(\partial_\tau f)(-\tau) = -\partial_\tau(f(-\tau))$ and $\int_{-a}^{a} d\tau[f(\tau) - f(-\tau)] = 0$ and the constancy of diagonal overlaps Eq. (6), one can recast Eq. (7) into the following forms:

$$
\begin{aligned}
S/\hbar &= -\int_{-T/2}^{T/2} d\tau \sum_k \langle\phi_k(\tau)|\partial_\tau[\phi_k(-\tau)]\rangle \\
&= \Re \int_{-T/2}^{T/2} d\tau \sum_k \langle\phi_k(-\tau)|\partial_\tau\phi_k(\tau)\rangle \\
&= 2\Re \int_{0}^{T/2} d\tau \sum_k \langle\phi_k(-\tau)|\partial_\tau\phi_k(\tau)\rangle. \qquad (13)
\end{aligned}
$$

The first equality shows that the action for instanton evolving backward in time, $\phi_k(-\tau)$, equals the minus action for the instanton. The second equality shows that the instanton action is a real number; the third one expresses action in terms of variables ϕ_{1k} and ϕ_{2k} defined by Eqs. (10).

Since $\partial_\tau|\phi_k\rangle = (\partial_\tau \ln|\phi_k|)|\phi_k\rangle + v$, with $v \perp |\phi_k(\tau)\rangle$, and $\phi_l(\tau)$ for all $l \neq k$ are perpendicular to $\phi_k(-\tau)$, the integrand $\langle\phi_k(-\tau)|\partial_\tau\phi_k(\tau)\rangle$ is the sum of the full derivative plus the contribution from the component $[\partial_\tau\phi_k]_\perp$ of the derivative $\partial_\tau\phi_k$ orthogonal to the subspace spanned by all vectors $\{\phi_k(\tau)\}_{k=1}^N$. After integration from $-T/2$ to $T/2$, only the latter contribution is left, that is,

$$S = \hbar \int_{-T/2}^{T/2} d\tau \sum_k \left\langle [\phi_k(-\tau)]_\perp \middle| \left[\frac{\partial\phi_k}{\partial\tau}(\tau)\right]_\perp \right\rangle, \qquad (14)$$

where $[\phi_k(-\tau)]_\perp$ is the component of $\phi_k(-\tau)$ perpendicular to $\{\phi_k(\tau)\}_{k=1}^N$. This shows that $[\phi_k(-\tau)]_\perp$ are the essential variables conjugate to $\phi_l(\tau)$, while the components of $\phi_k(-\tau)$ in the subspace $\{\phi_k(\tau)\}_{k=1}^N$ are completely fixed by the overlap constraints (6).

As bounce $\Phi(\tau)$ is a closed cycle in the Hilbert space $[\Phi(-\tau) \neq \Phi(\tau)$ unlike for a line segment], action S may be written in a form of the contour integral

$$S = \hbar \oint \sum_k \langle\phi_k(-\tau)|d\phi_k(\tau)\rangle, \qquad (15)$$

which manifests reparametrization invariance of S: it does not depend at all on the instanton "speed." As can be seen from Eq. (15), the only important features are the path traced by $|\phi_k\rangle$ in the vector space of s.p. states and the rule which associates pairs $\langle\phi_k(-\tau)|$ and $|\phi_k(\tau)\rangle$. Reparametrizations of imaginary time, $\tau \to \theta(\tau)$, which are both invertible $(d\tau/d\theta > 0)$ and consistent with the association rule $\tau(-\theta) = -\tau(\theta)$, $[\tau(-\Theta/2) = -T/2, \tau(\Theta/2) = T/2]$, leave S invariant. However, the reparametrized bounce, $\phi_k(\theta)$ is not a solution to Eqs. (3). Instead, it solves

$$\hbar\frac{\partial\phi_k}{\partial\theta}(\theta) + \frac{d\tau}{d\theta}(\hat{h}(\theta) - \epsilon_k)\phi_k(\theta) = 0. \qquad (16)$$

One can recover action if bounce is known up to a τ-dependent invertible linear transformation. Consider states $\psi_k(\tau)$ related to bounce $\phi_k(\tau)$ by means of such a transformation $N(\tau)$:

$$\phi_k(\tau) = \sum_l N_{lk}(\tau)\psi_l(\tau). \qquad (17)$$

Assume $N(\tau) = I$ at $\tau = \pm T/2$ and $\tau = 0$. Suppose that the overlaps $\langle\psi_k(-\tau)|\psi_l(\tau)\rangle$ are given by the matrix $M(\tau)$:

$$M_{kl}(\tau) = \langle\psi_k(-\tau)|\psi_l(\tau)\rangle, \qquad (18)$$

so that $M(-\tau) = M(\tau)^+$. The condition $\langle\phi_k(-\tau)|\phi_l(\tau)\rangle = \delta_{kl}$ means that

$$N^+(-\tau)M(\tau)N(\tau) = I, \qquad (19)$$

which leads to $M^{-1}(\tau) = N(\tau)N^+(-\tau)$. Calculate action in terms of states $\psi_k(\tau)$. The integrand is

$$
\begin{aligned}
&\sum_{ikl} N_{ki}^*(-\tau)\langle\psi_k(-\tau)|\partial_\tau[N_{li}(\tau)\psi_l(\tau)]\rangle \\
&\quad = \sum_{kl} M_{lk}^{-1}(\tau)\langle\psi_k(-\tau)\,|\,\partial_\tau\psi_l(\tau)\rangle + \sum_{il} N_{il}^{-1}(\tau)(\partial_\tau N_{li}(\tau)). \qquad (20)
\end{aligned}
$$

The second term is just $\mathrm{Tr}N^{-1}\partial_\tau N = \partial_\tau(\ln\det N)$. From Eq. (13) one obtains

$$S/\hbar = 2\Re\int_0^{T/2} d\tau \sum_{kl} M_{lk}^{-1}(\tau)\langle\psi_k(-\tau)|\partial_\tau\psi_l(\tau)\rangle, \tag{21}$$

where the omitted residual term, $\Re\int_{-T/2}^{T/2} d\tau\,\partial_\tau(\ln\det N(\tau))$ is identically zero, and the integration interval may be reduced to $[0, T/2]$ due to the properties of $M(\tau)$. Expanding either $\partial_\tau\psi_k(\tau)$ or $\psi_k(-\tau)$ onto $\psi_l(\tau)$ and a component perpendicular to all $\{\psi_k(\tau)\}_{k=1}^N$, one notices that only the part $[\partial_\tau\psi_k(\tau)]_\perp$ orthogonal to all $\psi_l(\tau)$ contributes to the action $S/\hbar = 2\Re\int_0^{T/2} d\tau \sum_{kl} M_{lk}^{-1}(\tau)\langle[\psi_k(-\tau)]_\perp|[\partial_\tau\psi_l(\tau)]_\perp\rangle$.

The Slater determinants $|\Psi(\tau)\rangle$, built out of $\psi_k(\tau)$, are related to bounce determinant states $|\Phi(\tau)\rangle$ by $|\Phi(\tau)\rangle = \det N(\tau)|\Psi(\tau)\rangle$, so that $\langle\Psi(-\tau)|\Psi(\tau)\rangle = \det M(\tau)$ and $\mathcal{H} = \langle\Phi(-\tau)|\ \ \hat{H}|\Phi(\tau)\rangle = \langle\Psi(-\tau)|\ \ \hat{H}|\Psi(\tau)\rangle/\langle\Psi(-\tau)|\ \ \Psi(\tau)\rangle$. Therefore, energy overlap kernel $\mathcal{H}$, like the action, does not involve $N(\tau)$ alone and may be expressed as [11]

$$\begin{aligned}\mathcal{H} &= \sum_i \langle\psi_i(-\tau)|\hat{t}|\psi_i'(\tau)\rangle \\ &\quad + \frac{1}{2}\sum_{i,j}\langle\psi_i(-\tau)\psi_j(-\tau)|\hat{v}|\psi_i'(\tau)\psi_j'(\tau) \\ &\quad - \psi_j'(\tau)\psi_i'(\tau)\rangle,\end{aligned} \tag{22}$$

where the states $\psi'(\tau)$ are related to $\psi(\tau)$ via $\psi_i'(\tau) = \sum_k M_{ki}^{-1}(\tau)\psi_k(\tau)$. The s.p. Hamiltonian $\hat{h}$ may be expressed in terms of various densities that do not involve $N(\tau)$ either, as, for example, $\rho(\tau) = \sum_i \psi_i^*(-\tau)\psi_i'(\tau) = \sum_k |\psi_k(\tau)|^2 + \sum_{kl} M_{kl}^{-1}(\tau)[\psi_l^*(-\tau)]_\perp\psi_k(\tau)$, etc. Equations (3) do involve $N(\tau)$:

$$\begin{aligned}&\hbar\partial_\tau\psi_k + \hat{h}\psi_k + \sum_l \hbar[(\partial_\tau N)N^{-1}]_{lk}\psi_l \\ &\qquad - \sum_l\left[\sum_m N_{lm}\epsilon_m N_{mk}^{-1}\right]\psi_l = 0.\end{aligned} \tag{23}$$

But they become independent of it when projected onto a space orthogonal to all $\{\psi_k(\tau)\}_{k=1}^N$:

$$(\hbar\partial_\tau\psi_k(\tau) + \hat{h}(\tau)\psi_k(\tau))_\perp = 0, \tag{24}$$

and only this part is relevant for action.

When the transformation $N(\tau)$ has the property of a "generalized unitarity," i.e., $N^{-1}(\tau) = N^+(-\tau)$, the overlaps of states $\psi_k(-\tau)$ and $\psi_l(\tau)$ have canonical form $M^{-1}(\tau) = N(\tau)N^+(-\tau) = I$. Then each of the matrices $N\epsilon N^{-1}$ and $(\partial_\tau N)N^{-1}$ has a Hermitian component that is τ-even and an anti-Hermitian component that is τ-odd. For an arbitrary nonsingular $N(\tau)$, in particular, one that keeps states $\psi_k(\tau)$ orthonormal, the matrix $M(\tau)$ in general depends on τ and has no defined τ parity. Conversely, a general form of the instanton equation

$$\hbar\partial_\tau\psi_k(\tau) + \hat{h}(\tau)\psi_k(\tau) + \sum_l \mathcal{E}_{lk}(\tau)\psi_l(\tau) = 0, \tag{25}$$

preserves the overlaps in Eq. (6) if $\mathcal{E}(\tau)$ has Hermitian τ-even and anti-Hermitian τ-odd parts. There is a great variety of possible instanton representations with different overlaps $\langle\psi_k(\tau)|\psi_l(\tau)\rangle$ corresponding to different matrices $\mathcal{E}$. The periodicity condition for instanton imposes integral conditions $\int_{-T/2}^{T/2} d\tau\,\partial_\tau(\langle\psi_k(\tau)|\psi_l(\tau)\rangle) = 0$, i.e., integral relations between the matrix elements of $\hat{h}_R$, $\mathcal{E}$, and the overlaps $\langle\psi_k(\tau)|\psi_l(\tau)\rangle$

$$\begin{aligned}&\int_{-T/2}^{T/2}\Big(2\langle\psi_k(\tau)|\hat{h}_R(\tau)|\psi_l(\tau)\rangle \\ &\qquad + \sum_m[\mathcal{E}_{mk}^*(\tau)\langle\psi_m(\tau)|\psi_l(\tau)\rangle + \langle\psi_k(\tau)|\psi_m(\tau)\rangle\mathcal{E}_{ml}(\tau)]\Big) \\ &\quad = 0.\end{aligned} \tag{26}$$

To ensure orthonormal $\{\psi_k\}$ at $\tau = 0$, both sets of integrals, $\int_0^{T/2}$ and $\int_{-T/2}^0$, should be zero. From Eqs. (3), we know that $\mathcal{E}_{kl} = -\epsilon_k\delta_{kl}$ provides one of the possible choices, but obviously there are many others, among them those with the diagonal matrix $\mathcal{E}$, i.e., with some τ-dependent s.p. energies $\epsilon_k(\tau)$.

For representations with orthonormal s.p. states $\psi_k(\tau)$, as for the usual HF determinants, Eq. (6) does not hold, while the following relations are satisfied: $\psi_k(-\tau) = \sum_i M_{ki}^*(\tau)\psi_i(\tau) + [\psi_k(-\tau)]_\perp$, and $\langle[\psi_k(-\tau)]_\perp|\ [\psi_l(-\tau)]_\perp\rangle = \delta_{kl} - (M(\tau)M^+(\tau))_{kl}$. Among them exists a special representation for which $\langle\psi_k(\tau)|\partial_\tau\psi_l(\tau)\rangle = 0$, which means that ∂_τ as an operator has only particle-hole (p-h) matrix elements. This corresponds to the matrix $\mathcal{E}$ which fulfills the equality $\mathcal{E} = -\hat{h}$ on the subspace spanned by $\{\psi_k(\tau)\}_{k=1}^N$.

IV. VARIATIONAL PRINCIPLE FOR BOUNCE ACTION

Consider variation of action S treated as a functional on trial fission paths defined in terms of s.p. states $\phi_{1k}(\tau)$ and $\phi_{2k}(\tau)$ for $0 < \tau < T/2$ as in Eq. (9), fulfilling instanton boundary conditions

$$\begin{aligned}\delta(S/\hbar) &= \sum_k\int_{-T/2}^{T/2}[(\langle\delta\phi_k(-\tau)|\partial_\tau\phi_k(\tau)\rangle \\ &\qquad - \langle\partial_\tau[\phi_k(-\tau)]|\delta\phi_k(\tau)\rangle] \\ &= \sum_k\int_0^{T/2}[\langle\delta\phi_{1k}(\tau)|\partial_\tau\phi_{2k}(\tau)\rangle \\ &\qquad - \langle\partial_\tau\phi_{1k}(\tau)|\delta\phi_{2k}(\tau)\rangle] + \text{c.c.}\end{aligned} \tag{27}$$

If the states ϕ_{2k} fulfill the first set of Eqs. (10) with ϕ_{1k} taken as the bra, then

$$\begin{aligned}\delta S &= \sum_k\int_0^{T/2}[\langle\delta\phi_{1k}(\tau)|\epsilon_k - \hat{h}(\tau)|\phi_{2k}(\tau)\rangle \\ &\qquad - \langle\hbar\partial_\tau\phi_{1k}(\tau)|\delta\phi_{2k}(\tau)\rangle] + \text{c.c.}\end{aligned} \tag{28}$$

If, additionally, energy is kept constant so that variations fulfill

$$\begin{aligned}\delta\mathcal{H} &= \sum_k[\langle\delta\phi_{1k}(\tau)|\hat{h}(\tau)\phi_{2k}(\tau)\rangle + \langle\hat{h}(-\tau)\phi_{1k}(\tau)|\delta\phi_{2k}(\tau)\rangle] \\ &= 0,\end{aligned} \tag{29}$$

then, since $\langle\phi_{1k}(\tau)|\phi_{2k}(\tau)\rangle = 1$, variation of S reads

$$\delta S = \sum_k \int_0^{T/2} \langle(\hat{h}(-\tau) - \epsilon_k)\phi_{1k}(\tau) - \hbar\partial_\tau\phi_{1k}(\tau)|\delta\phi_{2k}(\tau)\rangle + \text{c.c.} \quad (30)$$

As may be seen from this equation, after the first set of Eqs. (10) and the condition $\mathcal{H} = E_{\text{gs}}$ are fulfilled, action S ceases to be a functional of both ϕ_{1k} and ϕ_{2k} and becomes a functional of ϕ_{2k} and their time derivatives $\partial_\tau\phi_{2k}$. Through the s.p. Hamiltonian, the functions ϕ_{1k} provide the drive for ϕ_{2k} that is exactly required to produce $\partial_\tau\phi_{2k}$. As we have argued in Sec. II, and as follows from the physical meaning of action, for such a driven motion, S must be positive. Since $\delta S[\phi_{2k}]$ in Eq. (30) vanishes for ϕ_{1k} that fulfill the second set of instanton equations (10), i.e., when ϕ_{1k} and ϕ_{2k} together form the instanton, the instanton action must be a minimum of $S[\phi_{2k}]$. Thus, for ϕ_{2k} and ϕ_{1k} such that both fulfill the instanton boundary conditions, the overlap condition Eq. (6), the energy condition $\mathcal{H} = E_{\text{gs}}$ and ϕ_{1k} solve the first set of Eqs. (10) for $\partial_\tau\phi_{2k}$; the calculated action provides an upper bound for action of the optimal (i.e., the one with the smallest action, if there are a few) instanton. That the last condition is necessary may be seen from the negative sign of action for bounces evolving backward in τ, Eq. (13). The assumption that half of the bounce equations are fulfilled eliminates trial paths with admixtures of instantons evolving backward, which would leave the sign of action undecided. (Note that action for instanton evolving backward attains the maximal among negative values.) This is in complete analogy to mechanics, where the real motion $(q_i, \dot{q}_i)$ minimizes action $\int \sum_i p_i dq_i$ under the condition of constant energy *provided* that canonical relations $\dot{q}_i = \partial\mathcal{H}/\partial p_i$ are satisfied on each path. The variables introduced in the next section will make this analogy even closer.

One can use the principle of minimal action for any representation of a trial path. A simple choice is to take for ψ_{2k} some orthonormal HF states with the proper boundary conditions and to look for $[\psi_{1k}]_\perp$ such that $\langle\psi_{2l} \mid [\psi_{1k}]_\perp\rangle = 0$ and $\psi_{1k} = \psi_{2k} + [\psi_{1k}]_\perp$ fulfills Eq. (24) with some τ reparametrization as in Eq. (16), that is,

$$(\dot{\theta}\partial_\theta\psi_{2k} + \hat{h}[\psi_{1k}, \psi_{2k}]\psi_{2k})_\perp = 0. \quad (31)$$

In this representation, the overlap conditions are automatically fulfilled. Leaving τ reparametrization free, one gains a parameter $\dot{\theta}$ that allows one to control bounce velocity, i.e., the energy condition. One can decompose the s.p. mean-field Hamiltonian as suggested by the formula for density ρ preceding Eq. (23), $\hat{h}[\psi_{1k}, \psi_{2k}] = \hat{h}[\psi_{2k}] + \Delta\hat{V}[[\psi_{1k}]_\perp, \psi_{2k}]$, with $\hat{V}$ the s.p. potential, so that the equation for $[\psi_{1k}]_\perp$ becomes

$$-(\dot{\theta}\partial_\theta\psi_{2k} + \hat{h}[\psi_{2k}]\psi_{2k})_\perp = (\Delta\hat{V}[[\psi_{1k}]_\perp, \psi_{2k}]\psi_{2k})_\perp. \quad (32)$$

For complex wave functions, Eq. (32) should be solved together with its complex conjugate for both $[\psi_{1k}]_\perp$ and $[\psi_{1k}^*]_\perp$. For small $[\psi_{1k}]_\perp$, one could expand the right-hand side of this equation to linear terms in particle-hole components $[\psi_{1\perp}]_{ph}$ with respect to $\{\psi_{2h}\}$, $[\psi_{1h}]_\perp = \sum_p[\psi_{1\perp}]_{ph}|p\rangle$, and try to solve the system of linear equations with the matrix $\partial[\Delta\hat{V}\psi_{2h}]_p/\partial[\psi_{1\perp}^*]_{p'h'}$. This matrix, $\langle pp'|\hat{v}|\widetilde{hh'}\rangle$, where tilde means antisymmetrization, is the off-diagonal block of the RPA matrix (with respect to the HF state built of $\{\psi_{2h}\}$), which also appears in the ATDHF, cf. Eqs. (2.25)–(2.29) and (8.24) in Ref. [8], also Ref. [12]. The solution of Eq. (32) should be obtained for many velocities $\dot{\theta}$ to find the one that matches the energy condition. For larger barriers, larger differences between ψ_{1k} and ψ_{2k} are necessary to lower the energy overlap kernel $\mathcal{H}$ to E_{gs}. Then, the solution to Eq. (31) or (32) beyond the linear limit does not seem trivial. However, if found by any means, it provides action S as an upper bound for the decay exponent.

V. INSTANTONS IN COORDINATE-MOMENTUM VARIABLES

There are natural choices of instanton variables that correspond to time-even coordinates and time-odd momenta. One possibility is given [9] by $\phi_k(\tau) = \varphi_k(\tau) - \xi_k(\tau)$, $\phi_k(-\tau) = \varphi_k(\tau) + \xi_k(\tau)$. It follows that $\varphi_k(-\tau) = \varphi_k(\tau)$ and $\xi_k(-\tau) = -\xi_k(\tau)$. Because of the boundary conditions, $\varphi_k(\pm T/2) = \psi_k^{\text{HF}}$, $\varphi_k(0) = \phi_k(0)$, and $\xi_k(\pm T/2) = \xi_k(0) = 0$. Thus, φ_k are average tunneling states (coordinates) which may be parametrized by some deformation $Q(\tau)$ (or its real part, cf. Sec. II), so that $\partial_\tau\varphi_k = \dot{Q}\partial_Q\varphi_k$. The τ-odd components ξ_k must be proportional to the τ-odd derivative $\dot{Q}(\tau)$, i.e., the collective velocity. These two sets of states fulfill the system of equations

$$\hbar\frac{\partial}{\partial\tau}\begin{pmatrix}\varphi_k \\ \xi_k\end{pmatrix} = \begin{pmatrix}-\hat{h}_A & , \hat{h}_R - \epsilon_k \\ \hat{h}_R - \epsilon_k , & -\hat{h}_A\end{pmatrix}\begin{pmatrix}\varphi_k \\ \xi_k\end{pmatrix}, \quad (33)$$

where we have used decomposition $\hat{h}(\tau) = \hat{h}_R + \hat{h}_A$. These equations may be obtained either by decomposing Eqs. (3) or by deriving equations of motion from the functional $\int d\tau\langle\Phi(-\tau)|\hbar\partial_\tau + \hat{H}|\Phi(\tau)\rangle$ expressed by φ_k and ξ_k. In the latter case, one has to remember that $\varphi_k(-\tau)$ and $\xi_k(-\tau)$ no longer exist as independent variables. The canonical form of Eqs. (33), without the periodicity-fixing terms, is

$$\hbar\frac{\partial\varphi_k(\tau)}{\partial\tau} = -\frac{\delta\mathcal{H}}{\delta\xi_k^*(\tau)},$$
$$\hbar\frac{\partial\xi_k(\tau)}{\partial\tau} = \frac{\delta\mathcal{H}}{\delta\varphi_k^*(\tau)}, \quad (34)$$

with canonical pairs (φ_k, ξ_k^*) and (φ_k^*, ξ_k). Densities may be expressed in terms of φ_k and ξ_k, for example, one has $\rho(x) = \sum_k[|\varphi_k(x)|^2 - |\xi_k(x)|^2 - 2i\Im(\varphi_k^*(x)\xi_k(x))]$, etc. The conserved overlaps in terms of the amplitudes φ_k and ξ_k read

$$\langle\varphi_k|\varphi_l\rangle - \langle\xi_k|\xi_l\rangle = \delta_{kl},$$
$$\langle\varphi_k|\xi_l\rangle - \langle\xi_k|\varphi_l\rangle = 0. \quad (35)$$

The first set of Eqs. (33) is consistent with ξ_k being proportional to the collective velocity $\dot{Q}(\tau)$. In particular, $\hat{h}_A$ contains ξ_k in odd orders; for example, the anti-Hermitian component of the part $(-\mathbf{j}\cdot\nabla)$ of the Skyrme-type s.p. mean field is proportional to a piece $-[(\xi_i^*\nabla\varphi_i - \varphi_i^*\nabla\xi_i)/2 + \text{c.c.}]$ of the current density $\mathbf{j}$. The adiabatic limit corresponds to small $\dot{Q}$ and thus small $|\xi_k|$.

It may be seen that the instanton dependence on $\dot{Q}$ allows one to satisfy the bounce condition at $\tau = 0$. As $\xi_k = \dot{Q}\bar{\xi}_k$ with $\bar{\xi}_k$ τ-even, the time derivative in the second set of Eqs. (33), $\ddot{Q}\bar{\xi}_k + \dot{Q}^2\partial_Q\bar{\xi}_k$ reduces to $\ddot{Q}\bar{\xi}_k$ at $\tau = 0$, where $\dot{Q} = 0$ (we assume real Q). Then $\hat{h}_A(0) = 0$, so from the first set of Eqs. (33), $\bar{\xi}_k(0) = \left(\hat{h}(0) - \epsilon_k\right)^{-1}\partial_Q\varphi_k(0)$. Substituting this into the second set, we obtain the bounce condition at $\tau = 0$

$$\ddot{Q}\frac{\partial\varphi_k}{\partial Q}(0) = (\hat{h}(0) - \epsilon_k)^2\varphi_k(0), \tag{36}$$

where $\ddot{Q} = \frac{1}{2}d\dot{Q}^2/dQ$ is negative at $\tau = 0$, and $\dot{Q}^2$ is determined as a function of Q by the energy condition $\mathcal{H}[\varphi_k(Q), \dot{Q}\bar{\xi}_k(Q)] = E_{\rm gs}$. The exact Eq. (36) follows from the combined Eqs. (33) and therefore should not be imposed on trial paths in a variational search for instantons.

Because of the symmetry properties of the amplitudes, the action reads

$$S/\hbar = 2\Re\int_{-T/2}^{T/2} d\tau \sum_k \left\langle \xi_k \middle| \frac{\partial\varphi_k}{\partial\tau}\right\rangle. \tag{37}$$

In this expression, one immediately recognizes the familiar form $\int p_i dq_i$. The first set of Eqs. (33) are the velocity-momentum relations that should be fulfilled on trial trajectories in a search for bounce as a minimum of the action functional. Solving formally for momenta ξ_k and substituting into the action, one obtains

$$S = 2\hbar\int_{-T/2}^{T/2} d\tau \sum_k \left\langle \hbar\frac{\partial\varphi_k}{\partial\tau} + \hat{h}_A(\tau)\varphi_k \middle| \frac{1}{\hat{h}_R(\tau) - \epsilon_k} \middle| \frac{\partial\varphi_k}{\partial\tau}\right\rangle. \tag{38}$$

Let us compare this formula with a standard treatment of the spontaneous fission, in which one uses a family of static HF states, each constrained to have a prescribed quadrupole moment q, with values of q covering the barrier region. In such a study, one has to *assume* some form of the mass parameter $M(q)$ that allows one to express collective kinetic energy as $\frac{1}{2}M(q)\dot{q}^2$ and action as $\int M(q)\dot{q}dq$, with the implicitly understood energy conservation $V(q) - E_{\rm gs} = \frac{1}{2}M(q)\dot{q}^2$. In the cranking approximation, $M(q) = 2\hbar^2\sum_k\langle\partial\psi_k/\partial q|(\hat{h}_{\rm ad}(q) - e_k(q))^{-1}|\partial\psi_k/\partial q\rangle$, with the adiabatic mean-field Hamiltonian $\hat{h}_{\rm ad}$ and its eigenenergies e_k depending on q. After introducing a reparametrization $q(t)$ in terms of some "time" variable t to have the correspondence with Eq. (38), action in the cranking approximation can be written as

$$S_{\rm crank} = 2\hbar^2\int_{-T/2}^{T/2} dt \sum_k \left\langle \frac{\partial\psi_k}{\partial t} \middle| \frac{1}{\hat{h}_{\rm ad}(t) - e_k(t)} \middle| \frac{\partial\psi_k}{\partial t}\right\rangle. \tag{39}$$

One can see that Eq. (38), after neglecting the Thouless-Valatin term, is deceptively similar to the cranking expression. (The Thouless-Valatin term changes cranking masses by less than 20% [13].) However, a closer look reveals important differences: the constants ϵ_k in the denominator in Eq. (38) are the s.p. energies at the metastable HF minimum, not the adiabatic eigenenergies $e_k(q(t))$; the states φ_k, generally not orthonormal, are not equal to the adiabatic s.p. eigenstates $\psi_k(q(t))$; and the self-consistent s.p. Hamiltonian in the instanton method depends on τ-odd amplitudes, $\hat{h} = \hat{h}[\varphi_k, \xi_k]$, and this requires an iterative solution of the velocity-momentum relations.

As follows from Sec. III, ϵ_k could be replaced in the instanton Eqs. (10) and (33) by some τ-dependent quantities $\tilde{\epsilon}_k(\tau)$. Such a change results from scaling the s.p. bounce states via $\phi_k(\tau) = \phi_k'(\tau)\exp[\int_0^\tau(\epsilon_k - \tilde{\epsilon}_k(\tau'))d\tau'\hbar]$, with τ-even $\tilde{\epsilon}_k$. This is a particular linear transformation of the type in Eq. (17) which preserves the canonical overlaps [Eq. (6)] and the periodicity, if the conditions $\int_0^{T/2} d\tau\,\Delta\epsilon_k(\tau)/\hbar = 0$ are satisfied with $\Delta\epsilon_k = \epsilon_k - \tilde{\epsilon}_k(\tau)$. After such transformation, $\xi_k = \cosh(y)\xi_k' - \sinh(y)\varphi_k'$ with $y(\tau) = \int_0^\tau d\tau'\Delta\epsilon_k/\hbar$, so both ξ_k' and y have to be of the order $\dot{Q}$ to keep $\xi_k \sim \dot{Q}$ for small $\dot{Q}$. This requires that the average $\Delta\epsilon_k$ be of the order $\dot{Q}^2$, so only a mild deformation dependence of adiabatic energies is compatible with bounce properties.

A trial fission path is adiabatic if $\{\varphi_k\}$ differ only a little from orthonormal eigenstates of $\hat{h}_R$ with energies $\tilde{\epsilon}_k(\tau)$ obtained by such a rescaling, and the velocity-momentum relations produce small ξ_k. Then $\hat{h}_R[\varphi_k]$ may be considered the adiabatic mean field, and the cranking amplitudes ξ_k solve the second set of Eq. (35). This suggests (and will be shown by a different method in the next section) that in the adiabatic limit, $S_{\rm crank}$ provides an upper bound of Eq. (38) with the neglected Thouless-Valatin term.

Otherwise, when the larger ξ_k are required, the self-consistency and conditions in Eq. (35) induce a large difference between the contents of the cranking and instanton-motivated forms of action. For ξ_k not small, the enforcement of the velocity-momentum conditions together with Eq. (35) seems difficult. The same difficulty remains in the action minimization within this representation: since the properties of solutions to Eqs. (33) are not ensured for trial paths, the conditions for overlaps of Eq. (35) should be imposed on them independently of other necessary conditions.

VI. ADIABATIC LIMIT OF THE INSTANTON METHOD

A framework analogous to that of the ATDHF theory may be obtained by defining other variables. One can observe that because of the overlap conditions in Eq. (6), a linear transformation that maps each $\phi_k(\tau)$ into $\phi_k(-\tau)$ may be completed to a positive Hermitian operator. Denoting the square root of this operator at each τ as $\exp(\hat{S}(\tau))$, with $\hat{S}(\tau)$ Hermitian, we have $\exp(2\hat{S}(\tau))\phi_k(\tau) = \phi_k(-\tau)$ for all τ and k. Substituting $-\tau$ for τ in this relation and comparing both, we infer that $\hat{S}(-\tau) = -\hat{S}(\tau)$. Then, $\exp(\hat{S}(\tau))\phi_k(\tau) = \exp(\hat{S}(-\tau))\phi_k(-\tau)$ for all τ and k. This means that the above-defined vectors, which we will call $\psi_{0k}(\tau)$, are time-even and orthonormal. Thus we have

$$\phi_k(\tau) = \exp(-\hat{S}(\tau))\psi_{0k}(\tau),$$
$$\phi_k(-\tau) = \exp(\hat{S}(\tau))\psi_{0k}(\tau), \tag{40}$$

with $\psi_{0k}(\tau)$ some τ-even orthonormal states and $\hat{S}(\tau)$ a τ-odd operator. The relation of these new variables to those from the previous section is given by $\varphi_k = \cosh(\hat{S})\psi_{0k}$ and $\xi_k = \sinh(\hat{S})\psi_{0k}$. The condition $\hat{S}^+ = \hat{S}$ ensures the constant overlaps of Eq. (6). The bounce boundary conditions in terms of the new coordinates read $\psi_{0k}(\pm T/2) = \psi_k^{\rm HF}$, $\psi_{0k}(0) = \phi_k(0)$ and $\hat{S}(\pm T/2) = \hat{S}(0) = 0$. The states ψ_{0k} define a τ-even density matrix analogous to the ρ_0 of the ATDHF theory [12]. However, the object $e^{-\hat{S}}\rho_0 e^{\hat{S}}$ does not define any density matrix, contrary to $e^{i\hat{\chi}}\rho_0 e^{-i\hat{\chi}}$ of the ATDHF. The τ-odd matrix $\hat{S}$ must be proportional to $\dot{Q}(\tau)$. It introduces time-odd components to the s.p. wave functions, and its smallness is equivalent to the adiabaticity condition. The instanton equations may be written as

$$\hbar(e^{\hat{S}}(\partial_\tau e^{-\hat{S}})\psi_{0k} + \partial_\tau\psi_{0k}) + e^{\hat{S}}(\hat{h}(\tau) - \epsilon_k)e^{-\hat{S}}\psi_{0k} = 0. \tag{41}$$

Using expansions (with any operator $\mathcal{O}$)

$$e^{\hat{S}}\mathcal{O}e^{-\hat{S}} = \mathcal{O} + [\hat{S},\mathcal{O}] + \frac{1}{2!}[\hat{S},[\hat{S},\mathcal{O}]] + \frac{1}{3!}[\hat{S},[\hat{S},[\hat{S},\mathcal{O}]]] + \cdots,$$
$$e^{\hat{S}}(\partial_\tau e^{-\hat{S}}) = -\left(\partial_\tau\hat{S} + \frac{1}{2!}[\hat{S},\partial_\tau\hat{S}] + \frac{1}{3!}[\hat{S},[\hat{S},\partial_\tau\hat{S}]] + \cdots\right), \tag{42}$$

one can split Eq. (41) into τ-even and τ-odd parts. The equations so obtained are exact when the full expansion is kept. Since $\hat{h} = \hat{h}[e^{\hat{S}}\psi_{k0}, e^{-\hat{S}}\psi_{k0}]$, $\hat{h}_R(\tau)$ contains all even and $\hat{h}_A(\tau)$ all odd orders of $\hat{S}$. The approximation valid to the nth order in $\hat{S}$ consists in keeping the appropriate number of terms in both $\hat{h}_R$ and $\hat{h}_A$ in each term of the equations.

In the adiabatic limit, one expects that the time derivative introduces one order of smallness; so, for example, $\partial_\tau\hat{S}$ is of the order of $\hat{S}^2$. Then, up to the terms of the second order in $\hat{S}$ the equations read

$$\left(\hat{h}_R - \epsilon_k - \hbar\partial_\tau\hat{S} + \frac{1}{2}[\hat{S},[\hat{S},\hat{h}_0]] + [\hat{S},\hat{h}_A]\right)\psi_{0k} = 0,$$
$$\hbar\partial_\tau\psi_{0k} + \left([\hat{S},\hat{h}_0] + \hat{h}_A\right)\psi_{0k} = 0, \tag{43}$$

with the first order $\hat{h}_A$, and $\hat{h}_R$ of the order zero, equal to $\hat{h}_0 = \hat{h}[\psi_{0k}]$, except for the first term of the first equation, where the second order $\hat{h}_R$ should be used. In the time-odd equation, the lacking terms start at the order three and would include $-\frac{\hbar}{2}[\hat{S},\partial_\tau\hat{S}]\psi_{0k}$, etc. As discussed in the previous section, the difference between constants ϵ_k and the adiabatic energies $\epsilon_k(\tau)$, which may be understood as the expectation values $\langle\psi_{0k}|\hat{h}_0|\psi_{0k}\rangle$, resides in the diagonal part of $\partial_\tau\hat{S}$, generically of the order $\dot{Q}^2$. Clearly, not every static HF path is a proper candidate for τ-even bounce components ψ_{0k}, even if bounce is adiabatic (i.e. $\hat{S}$ is small).

In terms of ψ_{0k} and $\hat{S}$, action is given by

$$S/\hbar = \Re\int_{-T/2}^{T/2}\sum_k\langle\psi_{0k}|e^{\hat{S}}(\partial_\tau e^{-\hat{S}})|\psi_{0k}\rangle, \tag{44}$$

as the part of the integrand involving $\partial_\tau\psi_{0k}$ is identically zero because of the normalization of ψ_{0k}.

The approximation analogous to the ATDHF involves solving the second Eq. (43) up to the first order in $\hat{S}$. With a given Hamiltonian, energy up to the second order in $\hat{S}$ reads $\mathcal{H}_0 + \frac{1}{2}\langle\Psi_0|[\hat{S},[\hat{S},\hat{H}]]|\Psi_0\rangle$, with $\mathcal{H}_0 = \langle\Psi_0|\hat{H}|\Psi_0\rangle$. The term quadratic in $\hat{S}$ is negative and equal to $\mathrm{Tr}(\rho_0[\hat{S},[\hat{S},\hat{h}_0] + \hat{h}_A])/2$, with $\hat{h}_0 = \hat{h}[\rho_0]$ and $\hat{h}_A$ linear in $\hat{S}$. The latter operator is defined through its matrix elements between arbitrary states $|\alpha\rangle$ and $|\beta\rangle$ as

$$\langle\alpha|\hat{h}_A|\beta\rangle = \sum_k(\langle\alpha(\hat{S}\psi_{0k})|\hat{v}|\beta\widetilde{\psi_{0k}}\rangle - \langle\alpha\psi_{0k}|\hat{v}|\beta\widetilde{(\hat{S}\psi_{0k})}\rangle), \tag{45}$$

with the tilde denoting antisymmetrization. Up to the second order in $\hat{S}$, action is given by $S/\hbar = -\Re\int_{-T/2}^{T/2}\sum_k\langle\psi_{0k}|\partial_\tau\hat{S}|\psi_{0k}\rangle$, which may be expressed as

$$S/\hbar = 2\Re\int_{-T/2}^{T/2}\sum_k\langle\psi_{0k}|\hat{S}|\partial_\tau\psi_{0k}\rangle. \tag{46}$$

The lacking terms start at the order four, as the contribution of the order three, with the time-odd integrand $-\mathrm{Tr}(\rho_0[\hat{S},\partial_\tau\hat{S}])/2$, vanishes. After using the second Eq. (43), action in the adiabatic limit reads

$$S = -\int_{-T/2}^{T/2}d\tau\sum_k(\langle\psi_{0k}|\hat{S}(\hat{h}_A + [\hat{S},\hat{h}_0])|\psi_{0k}\rangle + \text{c.c.})$$
$$= -\int_{-T/2}^{T/2}d\tau\sum_k\langle\psi_{0k}|[\hat{S},\hat{h}_A + [\hat{S},\hat{h}_0]]|\psi_{0k}\rangle, \tag{47}$$

and hence is equal to the integral of $-\langle\Psi_0|[\hat{S},[\hat{S},\hat{H}]]|\Psi_0\rangle = -2(\mathcal{H} - \mathcal{H}_0)$.

If one has an energy functional instead of a Hamiltonian, one still obtains action (47). The integrand may be shown equal to $-2(\mathcal{H}[\varphi_k,\xi_k] - \mathcal{H}[\psi_{0k}])$, with $\varphi_k = (1+\hat{S}^2/2)\psi_{0k}$ and $\xi_k = \hat{S}\psi_{0k}$. One calculates $\delta\mathcal{H} = \mathcal{H}[\psi_{0k}+\delta\varphi_k, \xi_k + \delta\xi_k] - \mathcal{H}[\psi_{0k},\xi_k]$ for $\delta\varphi_k = \hat{S}^2\psi_{0k}/2$, $\xi_k = \hat{S}\psi_{0k}$ and $\delta\xi_k$ smaller than ξ_k, to the second order in $\hat{S}$ by using Eqs. (33) and (34) obtaining

$$\delta\mathcal{H} = \sum_k(\langle\delta\xi_k|\hat{h}_A(\tau)|\varphi_k\rangle - \langle\delta\xi_k|\hat{h}_0(\tau)|\xi_k\rangle + \langle\delta\varphi_k|\hat{h}_0(\tau)|\varphi_k\rangle + \text{c.c.}). \tag{48}$$

Then one deduces $\delta(\sum_k\langle\xi_k|\hat{h}_A|\varphi_k\rangle + \text{c.c.}) = 2(\sum_k\langle\delta\xi_k|\hat{h}_A|\varphi_k\rangle + \text{c.c.})$ and $\delta\langle\xi_k|\hat{h}_R|\xi_k\rangle = (\langle\delta\xi_k|\hat{h}_0|\xi_k\rangle + c.c)$ at the second order in $\hat{S}$. Thus, either with the Hamiltonian or the density functional, one obtains the same form of the positive integrand, which, when presented as $\dot{Q}^2\times$ mass, defines a positive mass for tunneling.

In ATDHF, the linear response limit of the time-odd equation, i.e., the counterpart of the second Eq. (43), is $\hbar\partial_\tau\psi_{0k} + (i\hat{h}_1 + [\hat{\chi},\hat{h}_0])\psi_{0k} = 0$, with $\hat{h}_0 = \hat{h}[\psi_{0k}]$, $\hat{h}_1 = i\mathrm{Tr}_2(\tilde{v}[\hat{\chi},\rho_0])$, $\tilde{v}$ is the antisymmetrized interaction, and Tr_2 indicates the trace over the coordinates of the second particle. However, $\hat{h}_1 = -i\hat{h}_A(\hat{\chi})$, so that the τ-odd equation for the instanton operator $\hat{S}$ is a copy of the ATDHF equation, with $\hat{S} = \hat{\chi}$. Thus, in the adiabatic limit, instanton action defines the ATDHF mass $\hbar\mathrm{Tr}(\hat{S}\dot{\rho}_0)/\dot{Q}^2$. In both cases, only the particle-hole components of $\hat{S}$ are determined.

The first Eq. (43) provides the adiabaticity condition for a trial path, as in ATDHF [8,12], but with a different sign by $\partial_\tau\hat{S}$. It is worth emphasizing, though, that this condition was practically never checked in calculations of ATDHF masses. Thus, up to now, decay probabilities were calculated without knowing whether a chosen fission path is compatible with this equation. As far as the action is concerned, the difference between the real- and imaginary-time dynamics, i.e., between oscillations and tunneling, appears in the next order.

A search for instanton in the adiabatic limit would consist in looking for the minimum of action calculated with the ATDHF mass over trial paths that should fulfill the adiabaticity condition. It is well known that near the s.p. level crossing at the Fermi surface, an extremely small velocity is needed to keep the occupation of the lower level. Since in ATDHF, $\dot{Q}$ must be also adjusted to keep the bulk energy $\mathcal{H}$ constant, it may fail to fulfill two requirements simultaneously in the vicinity of the crossing. Thus, the proper ATDHF fission path should avoid such crossings. Fission paths that break many symmetries, along which crossings are avoided by a strong interaction between levels, could provide one remedy for this problem (as suggested by the calculations reported in Ref. [3]). The other would be to solve Eq. (43) for instanton to the higher order in $\hat{S}$, which would modify the mean field $\hat{h}_R$ and avoid crossings present for the initial $\hat{h}_0$. Finally, a partial remedy is given by pairing.

VII. BOUNCE ACTION VS. GCM INERTIA

The use of the variational principle for instantons depends on the ability to impose the velocity-momentum conditions. These conditions are crucial, because without them action for a trial path may be lower than that for bounce. Below, we show that the GCM formula for a collective mass that restricts generating states to τ-even Slater determinants respects only the energy condition and hence is incompatible with the instanton method.

Consider a family of orthonormal states labeled by the quadrupole moments $q_1(\tau)$ and $q_2(\tau)$, $\tau > 0$, and calculate action Eq. (21). Through the barrier, $q_2(\tau)$ must be different from $q_1(\tau)$ to make the energy overlap kernel $\langle\Psi(q_1(\tau))|\hat{H}|\Psi(q_2(\tau))\rangle/\langle\Psi(q_1(\tau))|\Psi(q_2(\tau))\rangle$ equal to $E_{\rm gs}$. If we suppose that Ψ depends solely on q and not on $\dot{q}$, as in many GCM studies, the matrix $M(\tau)$ becomes a function of q_1 and q_2, the integrand in Eq. (21) becomes equal to $\mathrm{Tr}(M(q_1,q_2)^{-1}(\partial M(q_1,q_2))/\partial q_2)$, and

$$S = 2\hbar\Re\int_{q(0)}^{q(T/2)} dq_2 \frac{\partial \ln\det M(q_1,q_2)}{\partial q_2}. \quad (49)$$

From this equation, one can deduce a connection between the signs of S and $q_2 - q_1$: Eqs. (3) and (10) tell us that the deformation q_1 of the state $\Psi(q_1)$ drags deformation q_2 of $\Psi(q_2)$, thus q_2 lags behind q_1 on the way from behind the barrier to the metastable minimum, i.e., $q_2(\tau) > q_1(\tau)$. Therefore, increasing q_2 while keeping q_1 fixed *increases* separation between q_1 and q_2, and thus decreases the overlap $\det M(q_1,q_2)$. Hence, the integrand in Eq. (49) is negative, as is the differential dq_2 [as $q(0) > q(T/2)$], so action S is positive.

In the above reasoning, we used the property of the bounce equation. While using the variational principle, one might exchange the states Ψ_1 and Ψ_2, and then, by the previous reasoning, a negative action would follow. One might try to take $|S|$ for action in such a case, and there are cases in which this way of proceeding defines a minimum. At the same time, it is clear that some additional conditions are necessary in the variational formulation.

One can expand the integrand in Eq. (49) with respect to the quadrupole moment difference $s = q_2(\tau) - q_1(\tau)$ around the midpoint $\bar{q} = (q_1 + q_2)/2$. When one assumes the GOA, $\ln\det M(q_1,q_2) \approx -\gamma(\bar{q})s^2/2$, and then disregards quadratic and higher order terms in s, one obtains

$$S \approx -2\hbar\int_{q(0)}^{q(T/2)} dq_2\,\gamma(\bar{q})(q_2 - q_1), \quad (50)$$

where, as discussed above, $q_2 > q_1(q_2)$, and $\gamma(\bar{q}) = \sum_k\langle\partial_q\psi_k|\partial_q\psi_k\rangle - \sum_{kl}\langle\partial_q\psi_k|\psi_l\rangle\langle\psi_l|\partial_q\psi_k\rangle$. The integration variable $dq_2 = d\bar{q} + ds/2$ may be changed to $d\bar{q}$, as the integral $s\,ds = d(s^2)/2$ between the endpoints with $s = 0$ vanishes. The difference of the quadrupole moments may be calculated from the constraint on the energy overlap kernel: $E_{\rm gs} = \mathcal{H}[q_2,q_1] \approx \mathcal{H}[\bar{q},\bar{q}] - s^2(\mathcal{H}_{xy} - \mathcal{H}_{xx})/4$, where we have used the symbolic notation for derivatives of $\mathcal{H}$, e.g., $\mathcal{H}_{xx} = \partial_x^2\mathcal{H}(x,y)|_{x=y=\bar{q}}$, etc., and conditions $\mathcal{H}_x = \mathcal{H}_y$, $\mathcal{H}_{xx} = \mathcal{H}_{yy}$ holding for time-even $\mathcal{H}$ (cf. Ref. [14], where the discussion of those is given). Since the diagonal value of the energy overlap is just "potential energy" $V(\bar{q})$ in the standard approach, we obtain

$$S \approx 2\hbar\int_{q(T/2)}^{q(0)} d\bar{q}\sqrt{2(V(\bar{q}) - E_{\rm gs})\left(\frac{2\gamma(\bar{q})^2}{\mathcal{H}_{xy} - \mathcal{H}_{xx}}\right)}, \quad (51)$$

where the quantity in the second parenthesis under the square root sign is the GCM+GOA mass (cf. Ref. [14]).

Since additional constraints can only increase the minimum of a functional, the GCM mass must produce smaller action, and thus smaller decay exponent, than that of instanton. Any other action obtained with additional constraints will also produce a larger decay exponent. As the ATDHF respects the velocity-momentum conditions to the same order to which it is exact, it will produce larger S than the GCM. The results of calculations seem to support this, see, e.g., Refs. [15,16]. On the other hand, it is known that by introducing velocities (or momenta) as additional generating coordinates, one can show the equivalence of such a more general GCM and the ATDHF [8,17].

VIII. INCLUSION OF PAIRING IN THE INSTANTON METHOD

It is well known that the pairing interaction should be taken into account if realistic estimates for fission probabilities are to be found. In fact, it is pairing that gives the main contribution to the mass parameters, as it couples s.p. levels of different symmetries when they cross at the Fermi level. At the same time, it produces the gap in the quasiparticle spectrum which makes the collective motion more adiabatic. The proper self-consistent formalism to include pairing in the instanton approach is the HFB theory, in which the Slater determinants are replaced by the quasiparticle vacua, the many-particle states of undetermined particle number, annihilated by a set of operators

$$\alpha_i = \sum_{\mu}(A^*_{\mu i} a_\mu + B^*_{\mu i} a^+_\mu), \tag{52}$$

where operators a^+_μ refer to some fixed s.p. basis. We give here elements of the instanton method for systems with pairing. These include the imaginary-time version of the TDHFB equations, the counterpart of the formula Eq. (21) for action in terms of familiar HFB states, equations in coordinate-momentum variables [analogous to Eqs. (33)], and the formulation in terms of a time-even generalized density matrix and a time-odd Hermitian operator that leads naturally to the adiabatic limit.

For our purpose, it is helpful to notice that the above customary definition implies that the HFB vacuum $|\Psi\rangle \sim \exp(\frac{1}{2}\sum_{\mu\nu} Z_{\mu\nu} a^+_\mu a^+_\nu)|0\rangle$, with $Z = B^* A^{*-1}$, depends on matrices A^* and B^*, while $\langle\Psi|$, the corresponding bra, depends on A and B.

A. Imaginary-time TDHFB equations

The TDHFB theory is built on the condition of unitarity of the time-dependent Bogoliubov transformation and the variational principle. The HFB transformation for imaginary time, $t \to -i\tau$, becomes

$$\begin{pmatrix} \alpha^+(\tau) \\ \alpha(-\tau) \end{pmatrix} = \begin{pmatrix} A^T(\tau), & B^T(\tau) \\ B^+(-\tau), & A^+(-\tau) \end{pmatrix} \begin{pmatrix} a^+ \\ a \end{pmatrix}, \tag{53}$$

where $A(t)$ and $B(t)$ became functions of τ, while their complex conjugate $A^*(t)$ and $B^*(t)$ became functions of $-\tau$. The unitarity of the HFB transformation in the real-time formalism translates to the following condition in the imaginary-time version:

$$\begin{pmatrix} A^T(\tau), & B^T(\tau) \\ B^+(-\tau), & A^+(-\tau) \end{pmatrix}^{-1} = \begin{pmatrix} A^*(-\tau), & B(\tau) \\ B^*(-\tau), & A(\tau) \end{pmatrix}. \tag{54}$$

This equation means that fermionic anticommutation relations for operators a^+_μ, a_ν transfer to $\{\alpha_i(-\tau), \alpha_j(-\tau)\} = \{\alpha^+_i(\tau), \alpha^+_j(\tau)\} = 0$, and $\{\alpha_i(-\tau), \alpha^+_j(\tau)\} = \delta_{ij}$ (and *vice versa*). Denoting $\mathcal{N}(\tau)$ as the imaginary-time HFB transformation in Eq. (53), its properties may be concisely written as $\mathcal{N}^{-1}(\tau) = \mathcal{N}^+(-\tau) = \sigma_x \mathcal{N}^T(\tau)\sigma_x$, using the Pauli matrix notation for the block matrix. Written as separate conditions, these are eight matrix equations that reduce to four independent relations in which τ may be both positive or negative:

$$\begin{aligned} A^+(-\tau)A(\tau) + B^+(-\tau)B(\tau) &= I, \\ A^T(\tau)B(\tau) + B^T(\tau)A(\tau) &= 0, \\ A^*(-\tau)A^T(\tau) + B(\tau)B^+(-\tau) &= I, \\ A^*(\tau)B^T(-\tau) + B(-\tau)A^+(\tau) &= 0. \end{aligned} \tag{55}$$

The first of those differs from the usual HFB condition as it forces anticommutation between annihilation and creation operators of two different sets of τ and $-\tau$. This means that the usual relations $\{\alpha_i(\tau), \alpha^+_j(\tau)\} = \delta_{ij}$ are not ensured. However, as shown below, new operators related to $\alpha(\pm\tau)$ may be defined, fulfilling the usual conditions.

The variational principle that gives the TDHFB equations, transformed to imaginary time $t \to -i\tau$, becomes $\delta \int d\tau \langle\Phi(\tau)|\hbar\partial/\partial\tau + \hat{H}|\Phi(-\tau)\rangle = 0$. Calculating the variations $\delta/\delta A^*_{\mu i}(-\tau)$ and $\delta/\delta B^*_{\mu i}(-\tau)$, one has to use, as in the real-time case, the transformation conditions in Eq. (55) and account for the resulting redundancy of the variables A and B. The term with the time derivative that defines action becomes

$$\begin{aligned} S/\hbar &= \int d\tau \langle\Phi(\tau)|\partial_\tau \Phi(-\tau)\rangle \\ &= \frac{1}{2}\int d\tau \mathrm{Tr}[\partial_\tau A^+(-\tau)A(\tau) + \partial_\tau B^+(-\tau)B(\tau)] \\ &= -\frac{1}{2}\int d\tau \mathrm{Tr}[A^+(-\tau)\partial_\tau A(\tau) + B^+(-\tau)\partial_\tau B(\tau)]. \end{aligned} \tag{56}$$

The matrix element of the Hamiltonian $\langle\Phi(\tau)|\hat{H}|\Phi(-\tau)\rangle$ is expressed by the contractions

$$\begin{aligned} \langle\Phi(\tau)|a^+_\nu a_\mu|\Phi(-\tau)\rangle &= \rho_{\mu\nu}(\tau) = \left(B^*(-\tau)B^T(\tau)\right)_{\mu\nu}, \\ \langle\Phi(\tau)|a_\nu a_\mu|\Phi(-\tau)\rangle &= \kappa_{\mu\nu}(\tau) = \left(B^*(-\tau)A^T(\tau)\right)_{\mu\nu}, \\ \langle\Phi(\tau)|a^+_\nu a^+_\mu|\Phi(-\tau)\rangle &= \tilde{\kappa}_{\mu\nu}(\tau) = \left(A^*(-\tau)B^T(\tau)\right)_{\mu\nu}, \end{aligned} \tag{57}$$

which, due to conditions (55), have the following properties when regarded as matrices:

$$\begin{aligned} \rho(-\tau) &= \rho^+(\tau), \\ \kappa^T(\tau) &= -\kappa(\tau), \\ \tilde{\kappa}(\tau) &= \kappa^+(-\tau). \end{aligned} \tag{58}$$

Using those and proceeding as in the case of TDHFB, we arrive at the imaginary-time TDHFB equations written symbolically (where only the second index of the amplitudes is explicit):

$$\hbar\partial_\tau \begin{pmatrix} A_k(\tau) \\ B_k(\tau) \end{pmatrix} + \begin{pmatrix} \hat{t} + \hat{\Gamma}(\tau), & \hat{\Delta}(\tau) \\ -\hat{\Delta}^*(-\tau), & -(\hat{t} + \hat{\Gamma}(-\tau))^* \end{pmatrix} \begin{pmatrix} A_k(\tau) \\ B_k(\tau) \end{pmatrix} = E_k \begin{pmatrix} A_k(\tau) \\ B_k(\tau) \end{pmatrix}, \tag{59}$$

where, for a given Hamiltonian, the self-consistent potential $\Gamma_{\mu\nu}(\tau) = \sum_{\gamma\delta}(v_{\mu\gamma\nu\delta} - v_{\mu\gamma\delta\nu})\rho_{\delta\gamma}(\tau)$ and the pairing potential $\Delta_{\mu\nu}(\tau) = \sum_{\gamma\delta} v_{\mu\nu\gamma\delta}\kappa_{\gamma\delta}(\tau)$ have the properties $\hat{\Gamma}(-\tau) = \hat{\Gamma}^+(\tau)$ and $\hat{\Delta}^T(\tau) = -\hat{\Delta}(\tau)$. The same properties hold for the mean fields with additional rearrangement terms that follow from a density functional. These ensure the property $\hat{h}(-\tau) = \hat{h}^+(\tau)$ of the mean-field Hamiltonian $\hat{h}(\tau) = \hat{t} + \hat{\Gamma}(\tau)$, and the same property, $\hat{\mathbf{h}}(-\tau) = \hat{\mathbf{h}}^+(\tau)$ of the total HFB mean-field Hamiltonian $\hat{\mathbf{h}}(\tau)$ given by the matrix in Eqs. (59). As a result of this, Eqs. (59) conserves both energy and all relations in Eq. (55). The terms with constants E_k on the right-hand side fix the periodicity of solutions, and these constants are equal to the quasiparticle energies at the metastable HFB ground state. The bounce solution to Eqs. (59) has to be periodic and provide a path connecting the HFB ground state $|\Psi_{gs}\rangle$ with some HFB state $|\Phi(\tau=0)\rangle$ at the same energy beyond the barrier.

B. Variational principle

As in the HF case, one can deduce the minimum principle for action under conditions of constant energy and a fulfilled Eqs. (59) for $0<\tau<T/2$. The redundancy of variables A, B complicates the Hamilton equations, but the following relations hold: $-2\delta\mathcal{H} = \sum_k(\langle\delta\mathcal{W}_k(-\tau)\,|\,\hat{\mathbf{h}}(\tau)\,|\,\mathcal{W}_k(\tau)\rangle + \langle\mathcal{W}_k(-\tau)\,|\,\hat{\mathbf{h}}(\tau)|\delta\mathcal{W}_k(\tau)\rangle)$ and $-2\delta S = \hbar(\sum_k(\langle\delta\mathcal{W}_k(-\tau)|\partial_\tau\mathcal{W}_k(\tau)\rangle - \langle\partial_\tau[\mathcal{W}_k(-\tau)]$ $|\delta\mathcal{W}_k(\tau)\rangle)$, with $\mathcal{W}_k$ denoting the vector composed of (A_k, B_k). Since taking a formal variation of $S+\mathcal{H}$ with respect to $\delta\mathcal{W}_k^*$ and $\delta\mathcal{W}_k$ leads to the correct equations [Eqs. (59)], the arguments of Sec. IV can be repeated, and one obtains the same constraints that specify bounce as the minimum of action [note that $\langle\mathcal{W}_k(-\tau)|\mathcal{W}_l(\tau)\rangle = \delta_{kl}$].

The first equation in Eq. (55) means that $\langle\Phi(\tau)|\Phi(-\tau)\rangle = 1$. Since these two HFB states are different, the imaginary-time HFB transformation determined by the matrices $A(\pm\tau)$ and $B(\pm\tau)$ cannot be unitary. However, it may be related to a normal unitary HFB transformation given by some matrices $U(\tau), V(\tau)$ via some invertible, though nonunitary matrices $C(\tau)$. Let us suppose a relation

$$\alpha_i^+(\tau) = \sum_j C_{ji}(\tau)\beta_j^+(\tau), \tag{60}$$

with quasiparticle creation operators $\beta_i^+(\tau)$ related via some $U(\tau)$ and $V(\tau)$ matrices to a_μ^+, a_μ, namely [cf Eq. (53)],

$$\begin{pmatrix}\alpha^+(\tau)\\ \alpha(-\tau)\end{pmatrix} = \begin{pmatrix}(U(\tau)C(\tau))^T, & (V(\tau)C(\tau))^T\\ (V(-\tau)C(-\tau))^+, & (U(-\tau)C(-\tau))^+\end{pmatrix}\begin{pmatrix}a^+\\ a\end{pmatrix}. \tag{61}$$

It follows that $U(\tau), V(\tau)$ define the same $Z(\tau)$ as $A(\tau)$ and $B(\tau)$ do and that $U(\tau)^+U(\tau)+V(\tau)^+V(\tau) = C^{+-1}(\tau)(A^+(\tau)A(\tau)+B^+(\tau)B(\tau))C^{-1}(\tau)$. If one chooses $C(\tau)$ that transforms the Hermitian matrix $A^+(\tau)A(\tau) + B^+(\tau)B(\tau)$ to the unit matrix, then $U(\tau)$ and $V(\tau)$ become matrices of a standard HFB transformation. Now, the first equation of Eq. (55) means that

$$(U(-\tau)^+U(\tau)+V(-\tau)^+V(\tau))^{-1} = C(\tau)C(-\tau)^+, \tag{62}$$

while three other follow from this and from the HFB properties of matrices $U(\tau), V(\tau)$, and $U(-\tau), V(-\tau)$. The second equation in Eq. (55) is just the condition of the antisymmetry of $Z(\tau)$; the third and fourth equations, equivalent to $(I+Z^+(\tau)Z(-\tau))^{-1} + Z^+(\tau)(I + Z(-\tau)Z^+(\tau))^{-1}Z(-\tau) = I$ and the antisymmetry of matrices $Z(\tau)^+(I+Z(-\tau)Z^+(\tau))^{-1}$ and $(I+Z(-\tau)Z^+(\tau))^{-1}Z(-\tau)$, follow from the previous two.

Using the same reasoning as the one leading to Eq. (21), instanton action (56) can be expressed in terms of the normalized HFB states $|\Psi(\tau)\rangle$, defined by $U(\tau)$ and $V(\tau)$, using relation (62), as

$$S/\hbar = -\frac{1}{2}\Re\int_{-T/2}^{T/2} d\tau \mathrm{Tr}[(U^+(-\tau)U(\tau) + V^+(-\tau)V(\tau))^{-1}(U^+(-\tau)\partial_\tau U(\tau) + V^+(-\tau)\partial_\tau V(\tau))], \tag{63}$$

where we have omitted the integral of $\partial_\tau \ln\det C(\tau)$ between the endpoints, as it is purely imaginary.

The contractions in Eq. (58) can be expressed through $U(\pm\tau), V(\pm\tau)$ and the corresponding HFB states $\Psi(\pm\tau)$ in the following way:

$$\begin{aligned}\rho_{\mu\nu} &= (V^*(-\tau)(\tilde{U}(\tau)^T)^{-1}V^T(\tau))_{\mu\nu} = \frac{\langle\Psi(\tau)|a_\nu^+a_\mu|\Psi(-\tau)\rangle}{\langle\Psi(\tau)|\Psi(-\tau)\rangle},\\ \kappa_{\mu\nu} &= (V^*(-\tau)(\tilde{U}(\tau)^T)^{-1}U^T(\tau))_{\mu\nu} = \frac{\langle\Psi(\tau)|a_\nu a_\mu|\Psi(-\tau)\rangle}{\langle\Psi(\tau)|\Psi(-\tau)\rangle},\\ \tilde{\kappa}_{\mu\nu} &= (U^*(-\tau)(\tilde{U}(\tau)^T)^{-1}V^T(\tau))_{\mu\nu} = \frac{\langle\Psi(\tau)|a_\nu^+a_\mu^+|\Psi(-\tau)\rangle}{\langle\Psi(\tau)|\Psi(-\tau)\rangle},\end{aligned} \tag{64}$$

where the matrix $\tilde{U}(\tau) = U^+(-\tau)U(\tau) + V^+(-\tau)V(\tau)$ is related to the overlap of standard HFB states via $\langle\Psi(\tau)|\Psi(-\tau)\rangle = [\det\tilde{U}(\tau)]^{1/2}$ (see Ref. [14]).

Now, one can treat Eq. (63) as a functional on trial fission paths $\Psi(\tau)$, defined by two families of HFB states $\Psi_1(\tau)$ and $\Psi_2(\tau)$ for $0<\tau<T/2$

$$\Psi(\tau) = \begin{Bmatrix}\Psi_1(-\tau) \text{ for } \tau<0,\\ \Psi_2(\tau) \text{ for } \tau>0,\end{Bmatrix} \tag{65}$$

smoothly connecting some HFB state $\Phi(0)$ beyond the barrier at energy E_{gs} to the metastable ground state Ψ_{gs}, and fulfilling the condition of constant energy overlap and Eqs. (59) for $\Psi_2(\tau)$, that is $(\hbar\partial_\tau + \hat{\mathbf{h}}(\tau))\mathcal{W}_i(\tau) \perp \sigma_x\mathcal{W}_j^*(\tau)$ for all i, j, where $\mathcal{W}_k(\tau) = (U_{2k}(\tau), V_{2k}(\tau))$ correspond to quasiparticle states occupied in $\Psi_2(\tau)$. Taking $\tilde{U}(\tau) = U_1^+(\tau)U_2(\tau) + V_1^+(\tau)V_2(\tau)$ for $\tau>0$, and having $\tilde{U}(\tau) = \tilde{U}^+(-\tau)$ for $\tau<0$, one can calculate action as

$$S/\hbar = -\Re\int_0^{T/2} d\tau \mathrm{Tr}[\tilde{U}^{-1}(\tau)(U_1^+(\tau)\partial_\tau U_2(\tau) + V_1^+(\tau)\partial_\tau V_2(\tau))]. \tag{66}$$

The minimization of this action over fission paths that fulfill constraints should reproduce the bounce action. Its value for a trial path that satisfies constraints is an upper bound for the bounce decay exponent.

C. Coordinate and momentum variables

The coordinate-momentum variables may be introduced in a similar way as in Sec. V. Decomposing amplitudes into τ-even and τ-odd components, $A(\tau) = A_+(\tau) - A_-(\tau)$, $A(-\tau) = A_+(\tau) + A_-(\tau)$, $B(\tau) = B_+(\tau) - B_-(\tau)$, and $B(-\tau) = B_+(\tau) + B_-(\tau)$, with A_+ and B_+ matching Ψ_{gs} at $\tau = \pm T/2$ and $\Phi(0)$ at $\tau = 0$, and $A_- = B_- = 0$ at

$\tau = 0, \pm T/2$, one obtains the system of equations (with only the second index of the amplitudes made explicit)

$$\hbar\partial_\tau \begin{pmatrix} A_{+k} \\ B_{+k} \\ A_{-k} \\ B_{-k} \end{pmatrix} = \begin{pmatrix} -\hat{h}_A, & -\hat{\Delta}_-, & \hat{h}_R - E_k, & \hat{\Delta}_+ \\ -\hat{\Delta}_-^*, & -\hat{h}_A^*, & -\hat{\Delta}_+^*, & -\hat{h}_R^* - E_k \\ \hat{h}_R - E_k, & \hat{\Delta}_+, & -\hat{h}_A, & -\hat{\Delta}_- \\ -\hat{\Delta}_+^*, & -\hat{h}_R^* - E_k, & -\hat{\Delta}_-^*, & -\hat{h}_A^* \end{pmatrix} \times \begin{pmatrix} A_{+k} \\ B_{+k} \\ A_{-k} \\ B_{-k} \end{pmatrix}, \tag{67}$$

with the mean fields $\hat{h} = \hat{h}_R + \hat{h}_A$ and $\hat{\Delta} = \hat{\Delta}_+ + \hat{\Delta}_-$, with $\hat{\Delta}_+(-\tau) = \hat{\Delta}_+(\tau)$ and $\hat{\Delta}_-(-\tau) = -\hat{\Delta}_-(\tau)$. In a similar way as for Eqs. (33), the first two equations in Eqs. (67) connect velocities $\partial_\tau A_{+k}$, $\partial_\tau B_{+k}$ with momenta A_{-k} and B_{-k}, showing that they all, together with the τ-odd mean-field potentials $\hat{h}_A$ and $\hat{\Delta}_-$, are proportional to the collective velocity $\dot{Q}$. In the coordinate-momentum representation, these are the constraints that must be imposed on trial fission paths to ensure that bounce provides the minimum of the action functional. The relations in Eq. (55) written in terms of new amplitudes become eight relations that may be combined to four τ-even and four τ-odd equations, e.g., the first in Eq. (55) leads to $A_+^+A_+ - A_-^+A_- + B_+^+B_+ - B_-^+B_- = I$ and $A_-^+A_+ - A_+^+A_- + B_-^+B_+ - B_+^+B_- = 0$, etc.

Let us call the diagonal and off-diagonal submatrices of the matrix in Eqs. (67) $-\hat{\mathbf{h}}_A$ and $\hat{\mathbf{h}}_R$. From symmetries and definitions it is clear that $\hat{\mathbf{h}}_R(\tau)$ is Hermitian and time-even and $\hat{\mathbf{h}}_A(\tau)$ is anti-Hermitian and time-odd. In imaginary-time TDHFB, the operator $\hat{\mathbf{h}}_A$ is the generalization of the Thouless-Valatin mean field $\hat{h}_A$ of the ATDHF.

Denote the vector built of A_{+k} and B_{+k} as Θ_k and the one built of A_{-k} and B_{-k} as Ξ_k, i.e., $\mathcal{W}_k(\tau) = \Theta_k(\tau) - \Xi_k(\tau)$. Then Eqs. (67) take the form

$$\begin{aligned} \hbar\partial_\tau\Theta_k &= -\hat{\mathbf{h}}_A\Theta_k + (\hat{\mathbf{h}}_R - E_k)\Xi_k, \\ \hbar\partial_\tau\Xi_k &= (\hat{\mathbf{h}}_R - E_k)\Theta_k - \hat{\mathbf{h}}_A\Xi_k. \end{aligned} \tag{68}$$

The variation of energy written in terms of Θ_k and Ξ_k reads

$$2\delta\mathcal{H} = \sum_k (\langle\delta\Theta_k|\hat{\mathbf{h}}_A\Xi_k\rangle - \langle\delta\Theta_k|\hat{\mathbf{h}}_R\Theta_k\rangle - \langle\delta\Xi_k|\hat{\mathbf{h}}_A\Theta_k\rangle + \langle\delta\Xi_k|\hat{\mathbf{h}}_R\Xi_k\rangle + \text{c.c.}). \tag{69}$$

The three last terms, together with their complex conjugate, contribute at the second order in τ-odd components, assuming Ξ_k and $\delta\Xi_k$ being of the first, and $\delta\Theta_k$ of the second order of smallness. Owing to the τ parity of the amplitudes, and after integrating by parts, the action reads

$$S/\hbar = -2\Re\int_0^{T/2} d\tau \mathrm{Tr}[A_-^+(\tau)\partial_\tau A_+(\tau) + B_-^+(\tau)\partial_\tau B_+(\tau)]. \tag{70}$$

This can be expressed as $S = -\hbar\Re\int_{-T/2}^{T/2} d\tau \sum_k \langle\Xi_k|\partial_\tau\Theta_k\rangle$, i.e., it is imaginary-time TDHFB action in the form $\int p_i\, dq_i$. Substituting Ξ_k from the first Eq. (68), one can obtain the cranking-like expression for action as in Sec. V.

D. Adiabatic expansion and limit

The above formulas are a copy of those in Secs. V and VI, up to the common factor $(-1/2)$ appearing in the expressions for S and $\delta\mathcal{H}$. Hence, after showing that the operator that maps amplitudes at τ onto those at $-\tau$ is Hermitian, one could represent HFB bounce in terms of τ-even amplitudes and a τ-odd Hermitian operator $\hat{S}$, as in Sec. VI, and repeat the whole reasoning on the adiabatic limit of the instanton method. (To emphasize the analogy, we keep the same notation for the time-odd operator as in HF, although it acts in the enlarged space.)

The argument goes as follows: The HFB transformation from operators $(\alpha^+(\tau), \alpha(-\tau))$ to $(\alpha^+(-\tau), \alpha(\tau))$ is $\mathcal{N}(-\tau)\mathcal{N}^{-1}(\tau) = \mathcal{N}(-\tau)\mathcal{N}^+(-\tau)$ [cf. Eq. (54)], indeed Hermitian and positive. Calling this transformation $\exp(2\mathcal{S}(\tau))$, with $\mathcal{S}(\tau)$ Hermitian, and considering its inverse, we have $\mathcal{S}(-\tau) = -\mathcal{S}(\tau)$. Then, we find that $\exp(\mathcal{S}(\tau))\mathcal{N}(\tau) = \exp(\mathcal{S}(-\tau))\mathcal{N}(-\tau)$; calling this τ-even transformation $\bar{\mathcal{N}}(\tau)$, we have $\bar{\mathcal{N}}^{-1}(\tau) = \bar{\mathcal{N}}^+(\tau)$, so $\bar{\mathcal{N}}(\tau)$ is a regular HFB transformation. Denoting its amplitudes u and v, we have

$$\begin{pmatrix} A^T(\tau), & B^T(\tau) \\ B^+(-\tau), & A^+(-\tau) \end{pmatrix} = \exp(-\mathcal{S}(\tau))\begin{pmatrix} u^T(\tau), & v^T(\tau) \\ v^+(\tau), & u^+(\tau) \end{pmatrix}. \tag{71}$$

The properties of $\mathcal{N}(\tau)$ and $\bar{\mathcal{N}}(\tau)$ imply $\sigma_x\mathcal{S}^T(\tau)\sigma_x = -\mathcal{S}(\tau)$. As we need a relation between amplitudes and these form columns of the matrices $\mathcal{N}^T(\tau)$ and $\bar{\mathcal{N}}^T(\tau)$, we notice that $\mathcal{N}^T(\tau) = [\bar{\mathcal{N}}^T(\tau)\exp(-\mathcal{S}^T(\tau))(\bar{\mathcal{N}}^T)^{-1}(\tau)]\bar{\mathcal{N}}^T(\tau)$ and that the matrix $\bar{\mathcal{N}}^T(\tau)\exp(-\mathcal{S}^T)(\tau))(\bar{\mathcal{N}}^T)^{-1}(\tau)$ is Hermitian owing to the HFB property of $\bar{\mathcal{N}}(\tau)$. Moreover, due to this property, one has $\mathcal{N}^T(\tau) = \exp(-\hat{S}(\tau))\bar{\mathcal{N}}^T(\tau)$ with the Hermitian, τ-odd $\hat{S}(\tau) = \bar{\mathcal{N}}^T(\tau)\mathcal{S}^T(\tau)\bar{\mathcal{N}}^*(\tau)$. It follows from the properties of $\mathcal{N}$ and $\mathcal{S}$ that $\sigma_x\hat{S}^T(\tau)\sigma_x = -\hat{S}(\tau)$. Thus

$$\hat{S} = \begin{pmatrix} \hat{s}, & \hat{r} \\ -\hat{r}^*, & -\hat{s}^* \end{pmatrix}, \tag{72}$$

with $\hat{s}^+ = \hat{s}$, and $\hat{r}^T = -\hat{r}$. With this $\hat{S}(\tau)$, we have the expected relations

$$\begin{aligned} \begin{pmatrix} A_k(-\tau) \\ B_k(-\tau) \end{pmatrix} &= \exp(\hat{S}(\tau))\begin{pmatrix} u_k(\tau) \\ v_k(\tau) \end{pmatrix}; \\ \begin{pmatrix} A_k(\tau) \\ B_k(\tau) \end{pmatrix} &= \exp(-\hat{S}(\tau))\begin{pmatrix} u_k(\tau) \\ v_k(\tau) \end{pmatrix}, \end{aligned} \tag{73}$$

where only the second index of the amplitudes is shown. With these, all the results of Sec. VI can be repeated for imaginary-time TDHFB. In particular, the integrand of the action integral S, which in terms of the amplitudes $\mathcal{W}_{0k} = (u_k, v_k)$ and the operator $\hat{S}$ reads $-\frac{\hbar}{2}\sum_k(\langle\partial_\tau\mathcal{W}_{0k}|\hat{S}|\mathcal{W}_{0k}\rangle + \text{c.c.})$, is equal to $-2(\mathcal{H} - \mathcal{H}_0)$ at the second order in $\hat{S}$, hence it is positive. Equations (59) take exactly the form of Eq. (41) of the imaginary-time TDHF, with obvious replacements of $\mathcal{W}_{0k}$ for

ψ_{0k} and $\hat{\mathbf{h}}$ for $\hat{h}$. They reduce to the form of Eq. (43) at the second order in $\hat{S}$.

The TDHFB equations may be also formulated in terms of the generalized density matrix. The counterpart of the HFB density matrix in the imaginary-time formalism is

$$\begin{aligned}&\begin{pmatrix}\rho(\tau), & \kappa(\tau)\\ -\kappa^*(-\tau), & I-\rho^*(-\tau)\end{pmatrix}\\ &=\begin{pmatrix}B^*(-\tau)\\ A^*(-\tau)\end{pmatrix}(B^T(\tau), A^T(\tau))\\ &=[\sigma_x \exp(\hat{S}^*(\tau))\sigma_x]\mathcal{R}_0(\tau)[\sigma_x \exp(-\hat{S}^T(\tau))\sigma_x], \qquad (74)\end{aligned}$$

with $\mathcal{R}_0(\tau)$ the HFB density matrix corresponding to $\bar{\mathcal{N}}(\tau)$. Owing to the property of $\hat{S}$, it is equal to $e^{-\hat{S}(\tau)}\mathcal{R}_0(\tau)e^{\hat{S}(\tau)}$. This non-Hermitian quantity, call it $\widetilde{\mathcal{R}}$, apart from not being a HFB density matrix, is an analog (note that $\widetilde{\mathcal{R}}^2=\widetilde{\mathcal{R}}$) of the density matrix in the ATDHFB theory [18], $\mathcal{R}=e^{i\hat{\chi}}\mathcal{R}_0e^{-i\hat{\chi}}$. In terms of it, Eqs. (59) reads $\hbar\partial_\tau\widetilde{\mathcal{R}}+[\hat{\mathbf{h}},\widetilde{\mathcal{R}}]=0$. The τ-odd part of this equation, linear in $\hat{S}$, obtained by expanding $\widetilde{\mathcal{R}}=\mathcal{R}_0-[\hat{S},\mathcal{R}_0]+\cdots$ and discarding the second-order quantity $[\hat{\mathbf{h}}_0,\mathcal{R}_0]$, is

$$\hbar\partial_\tau\mathcal{R}_0+[[\hat{S},\hat{\mathbf{h}}_0]+\hat{\mathbf{h}}_A,\mathcal{R}_0]=0, \qquad (75)$$

which is an alternative form of the second Eq. (43) in terms of $\mathcal{R}_0$ and $\hat{S}$. Its solution is identical to the ATDHFB solution, $\hat{S}=\hat{\chi}$. This follows directly from the structure of the building blocks of the Thouless-Valatin mean field $\hat{\mathbf{h}}_A$. One has $\hat{h}_A=\mathrm{Tr}(\tilde{v}\rho_1)$ and $\Delta_{-\alpha\beta}=\sum_{\gamma\delta}v_{\alpha\beta\gamma\delta}\kappa_{1\gamma\delta}$, with $\rho_1=-[\hat{s},\rho_0]+\hat{r}\kappa_0^*-\kappa_0\hat{r}^*$, $\kappa_1=\rho_0\hat{r}+\hat{r}(\rho_0^*-1)-\hat{s}\kappa_0-\kappa_0\hat{s}^*$. Since, in ATDHFB, $\mathcal{R}_1=i[\hat{\chi},\mathcal{R}_0]$, one has $\hat{\mathbf{h}}_A=i\hat{\mathbf{h}}_1$, where $\hat{\mathbf{h}}_1$ is the ATDHFB time-odd mean field for $\hat{\chi}=\hat{S}$. Thus, the adiabatic TDHFB instanton method produces mass given by mass $\times\dot{Q}^2=\frac{\hbar}{2}\mathrm{Tr}(\dot{\mathcal{R}}_0\hat{S})$, equal to the ATDHFB mass, cf. Ref. [19]. In the zero pairing limit this mass reduces to the ATDHF value $\hbar\mathrm{Tr}(\dot{\rho}_0\hat{s})/\dot{Q}^2$.

A reasoning similar to the one presented in Sec. VII shows that within the GCM approach, a use of some τ-even pairing variable (for example, the pairing gap) as a generator coordinate, without fulfilling the velocity-momentum relations, will lead to a smaller decay exponent than that for bounce.

IX. CONCLUSIONS

We have presented the instanton method for nuclear fission in various representations. This has allowed us to make some comparisons with other methods commonly used in fission studies. We have also sketched the imaginary-time version of the TDHFB theory, which allows us to include pairing.

There are many similarities between the instantons describing quantum tunneling and the periodic TDHF solutions. Both appear as a result of the quasiclassical approximation, find a natural formulation in terms of time-even coordinates and time-odd momenta, and reduce to the same time-odd ATDHF equation in the lowest order in momenta. The ATDHF equation for a path, in particular, the smallness of $[\hat{h}_0,\rho_0]$, is usually not checked for static paths constructed by means of the CHF. When the velocity-momentum equations require large momenta, the chosen path is far from instanton.

The main difference between the two methods is that in quantum tunneling there is no single HF state or density matrix, but one deals with two different states, bra and ket. This happens to be the very reason for the existence of the minimum principle: it defines the minimal driving of one state by the other, necessary for tunneling. Instanton action turns out to be a minimum of the action functional when the constraints of constant energy and velocity-momentum relations are imposed on trial fission paths. Action calculated for any such path would provide an upper bound for the decay exponent. We argue that the ATDHF (ATDHFB) mass respects those constraints, while the GCM+GOA mass does not. The main practical problem is how to construct trial paths fulfilling the constraints.

The need for two Slater determinants for instanton leads to another important difference between the mean-field studies of oscillations and quantum tunneling: the instanton method relies on the off-diagonal matrix elements of the Hamiltonian, which are beyond the usual scope of the mean-field theory. To use instantons in practice, one has to define various off-diagonal matrix elements of the commonly used effective interactions. These include the density-dependent term of the Skyrme-like force (for its possible definitions, see Ref. [20]) and the Coulomb-exchange interaction.

When comparing the instanton method to theories of large amplitude collective motion (LACM) one has to recognize that the aims of the latter are much wider than those of the former [17,21]. In LACM, equations for the collective path or action are a source of formulas for potential and inertia tensor of an effective Hamiltonian in a restricted set of deformation coordinates and conjugate momenta. Often the next step consists in the requantization. The supposed universality of the so-conceived effective theory for LACM underlies the whole procedure. On the contrary, instanton should be found once for a studied decay. No interpretation of the integrand in the action formula as mass $\times\dot{Q}^2$ is necessary. It could be even dangerous, as in some representations of instanton these integrands are piecewise negative. Only the value of the integral has physical significance, and this does not depend on the representation.

Of course, one could extract collective inertia from action represented with a positive integrand, but the positivity is obvious only in the adiabatic limit. In a general case, the action in Eq. (38) contains momenta ξ_k to all even orders, and the higher order terms become naturally more important for higher barriers. Hence one expects that mass also depends on the barrier height, or energy, when tunneling from excited states is considered. A small energy dependence of mass is seen even for the highly collective Bose-Einstein condensate [7].

For pairing gaps of $\sim$1 MeV and for not too high fission barriers, the adiabatic approximation may be satisfactory for many fission paths. Then it may appear that the most important in the search for instanton is the exploration of a sufficiently rich family of paths, preferably with as few preserved symmetries as possible, while ATDHFB action (including Thouless-Valatin terms) is a sufficient estimate of the instanton action.

Even if this is true, fission of odd-Z or odd-N nuclei will require much more effort to understand, within the instanton method, a dramatic significance of the odd fermion and of the specific mean fields induced by it that break time-reversal invariance.

It is clear that the method considered here is applicable to quantum tunneling in any fermion system, provided it has a meaningful mean-field description. Extensions to include thermal effects and decay from excited states seem also straightforward. The real progress of the method will depend on practical solutions.

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