Nuclear fission with mean-field instantons

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We consider a variational search for instantons - imaginary-time mean fields, describing spontaneous fission, and generally quantum tunneling, within the mean-field theory. A formula for the decay exponent is given in terms of trial Hartree-Fock states. Exact for an instanton, it requires additional conditions to be imposed on trial paths to provide an upper bound for the instanton action.

1. A fair, and often the only one feasible, description of systems including hundreds or more particles relies on quantum mean-field theory. Unhappily, such theory does not contain quantum tunneling. Specifically, as the Hartree-Fock (HF) equations give only minima of the Hamiltonian

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

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

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

with $\hat{h}(t)\psi(t) = \delta\mathcal{H}/\delta\psi^*(t)$ and $\delta\mathcal{V}/\delta\psi_k^*(t) = \hat{V}(t)\psi_k(t)$, $\hat{h}(t)$ and $\hat{V}(t)$ being the single-particle (s.p.) mean-field Hamiltonian and potential, respectively. The Hamiltonian (1) and overlaps $\langle\psi_k \mid \psi_l\rangle$ are conserved by Eq. (2). The former forbids any tunneling within TDHF.

2. A method to include quantum tunneling in the mean-field description of a many-body system has been formulated in [1]. It exploits an idea of trajectories evolving in imaginary time [2] which emerge from the stationary-phase approximation to the path integral expression for $Tr(E-\hat{H})^{-1}$. 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 a prefactor coming from fluctuations around the optimal path.)

For one particle such optimal imaginary-time trajectory leaves the ground state and returns there after bouncing back from the inverted potential; hence the name 'bounce'. For a system of interacting fermions, one has to transform TDHF Eq. (2) to imaginary time, i.e., formally, $t \to -i\tau$. Under this transformation, $\psi \to \psi(x,-i\tau) = \phi(x,\tau)$ and $\psi^* \to \psi(x,-i\tau)^* = \phi(x,-\tau)^*$ [3, 4]. 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]:

$$\hbar\frac{\partial\phi_k}{\partial\tau}(\tau) = -\left(\hat{h}[\phi^*(-\tau);\phi(\tau)] - \epsilon_k\right)\phi_k(\tau) = \frac{\hbar^2}{2m}\nabla^2\phi_k(\tau) - \frac{\delta\mathcal{V}}{\delta\phi_k^*(-\tau)} + \epsilon_k\phi_k(\tau), \tag{3}$$

are non-local in time, as $\mathcal{V}$ depends on both $\phi(x,\tau)$ and $\phi(x,-\tau)$. Second, density $\rho(x,\tau)$ may be piecewise negative or complex. In analogy with TDHF, Eq. (3) conserve energy $\mathcal{H}$, with:

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

The mean-field Hamiltonian $\hat{h}(\tau)$, defined by $\hat{h}(\tau)\phi(\tau) = \delta\mathcal{H}/\delta\phi^*(-\tau)$, fulfills the condition $\hat{h}(-\tau) = \hat{h}^+(\tau)$, which ensures that Eq. (3) *without the* $\epsilon_k\phi_k$ *term*, conserve the overlaps: $d/d\tau\langle\phi_i(-\tau) \mid \phi_j(\tau)\rangle = 0$. The complete Eq. (3) still conserve diagonal overlaps, while giving the exponential time-dependence to the off-diagonal ones. However, those overlaps remain zero, if equal zero at some τ. The purpose of the $\epsilon_i\phi_i$ terms in the Eq. (3) is to assure the periodicity of solutions $\phi_k(\tau)$: $\phi_k(T/2) = \phi_k(-T/2)$, dictated by the saddle point approximation to the path integral. For the decay of a metastable ground state, boundary conditions must be completed by specifying the initial (and thus also the final) states as the HF solutions at the metastable minimum, $\phi_k(T/2) = \phi_k(-T/2) = \psi_k^{HF}$, with total energy E_{gs} and s.p. energies ϵ_k. States $\phi_k(\tau = 0)$ form some normal (as $\phi_k^*(-\tau) = \phi_k^*(\tau)$ at $\tau = 0$) HF state at energy E_{gs} on "the other side of the barrier". The periodicity condition together with the initial condition fix the particular constant values of the overlaps: $\langle \phi_i(-\tau) \mid \phi_j(\tau)\rangle = \delta_{ij}$.

Decay exponent is given by [1]:

$$S = \hbar \int_{-T/2}^{T/2} d\tau \sum_k \langle \phi_k(-\tau) \mid \frac{\partial \phi_k}{\partial \tau}(\tau)\rangle. \tag{5}$$

Bounce penetrates the static barrier, 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]. Eq. (3) determine both decay channels and decay probabilities.

By using the general identities: $(\partial_\tau f)(-\tau) = -\partial_\tau(f(-\tau))$, $\int_{-a}^{a} d\tau[f(\tau) - f(-\tau)] = 0$, and the constancy of diagonal overlaps one can recast Eq. (5) into the following form:

$$S/\hbar = -\int_{-T/2}^{T/2} d\tau \sum_k \langle \phi_k(\tau) \mid \partial_\tau[\phi_k(-\tau)]\rangle = 2\Re \int_{-T/2}^{0} d\tau \sum_k \langle \phi_k(-\tau) \mid \partial_\tau \phi_k(\tau)\rangle. \tag{6}$$

Thus, action is real and determined by the instanton on $[-T/2, 0]$.

3. To obtain equations local in time, one can present s.p. wave functions as [4]: $\phi_k = \sqrt{\rho_k}\exp(-\chi_k)$, whith ρ_k time-even, and χ_k time-odd. For one real wave function, and potential energy being a functional of density, $\mathcal{V}[\rho]$, one can split Eq. (3) into continuity and "fluid velocity" parts, as for the density-phase representation of the Schrödinger equation. The energy $\mathcal{H}$ becomes:

$$\mathcal{H} = \frac{\hbar^2}{m} \int dx \left[-\frac{\rho(\nabla\chi)^2}{2} + \frac{(\nabla\rho)^2}{8\rho}\right] + \mathcal{V}[\rho], \tag{7}$$

where the minus sign shows the role of χ in lowering the HF energy down to E_{gs} in the barrier region. Using the boundary conditions, symmetries of ρ and χ, and the continuity equation, one gets:

$$S = -\hbar \int_{-T/2}^{T/2} d\tau \int dx \rho \partial_\tau \chi = \frac{\hbar^2}{m} \int_{-T/2}^{T/2} d\tau \int dx \rho (\nabla\chi)^2. \tag{8}$$

or, equivalent: $S = 2\int_{-T/2}^{T/2} d\tau T_{coll}(\tau)$ if one identifies the collective kinetic energy as $T_{coll}(\tau) = \hbar^2/(2m) \times \int dx \rho_(\nabla\chi)^2$. With this formula, one can describe a collapse of the Bose-Einstein condensate of ^{7}Li atoms which at sufficiently low temperature proceeds via macroscopic quantum tunneling [5]. For radially symmetric condensate, it is even possible to express χ as a functional of ρ and obtain action as a functional of density, which can be then minimized in order to find instanton [6].

Since the velocity potential $\chi = -\frac{1}{2}(\ln\phi(\tau) - \ln\phi(-\tau))$ is regular only for ϕ_k having τ-symmetric zeroes, this procedure becomes questionable for $\rho(\tau)$ negative. It does not seem promising for fermions, for which there are four, not two, equations per each particle due to the spinor structure, and nodes of many ϕ_k rearrange at s.p. level crossings along the barrier. Moreover, in spite of the local-in-time representation of Eq. (3), the boundary conditions, which mean inverse diffusion for $0 < \tau < T/2$, make their solution very difficult [7].

Therefore, we try to advance a variational approach to finding S, hoping that a good estimate of action may be easier to find than that of the instanton itself. We consider a trial tunneling path as two sets of wave functions, $\{\phi_{1k}(\tau)\}$ and $\{\phi_{2k}(\tau)\}$, defined on the interval $[-T/2, 0]$, which determine the whole instanton as:

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

We suppose that the boundary conditions are fulfilled. For two Slater determinants, $\Phi(\tau)$ built out of $\phi_k(\tau)$, and $\Phi(-\tau)$ built out of $\phi_k(-\tau)$, the overlap condition for the instanton, $\langle \phi_k(-\tau) \mid \phi_l(\tau)\rangle = \delta_{kl}$, simply means $\langle \Phi(-\tau) \mid \Phi(\tau)\rangle = 1$, the energy conservation Eq. (4) means that $\langle \Phi(-\tau) \mid \hat{H} \mid \Phi(\tau)\rangle = E_{gs}$.

4. One can observe that action S relies only on a part of information contained in the bounce solution. The formula for S may be written in a form:

$$S = \oint \sum_k \langle \phi_k(-\tau) \mid d\phi_k(\tau)\rangle, \tag{10}$$

which manifestly shows that S does not depend at all on the instanton "speed". As can be seen from Eq. (10), the only important features are: the path traced by $\mid \phi_k\rangle$ in the vector space of s.p. states and the rule which associates pairs $\langle\phi_k(-\tau)\mid$ and $\mid\phi_k(\tau)\rangle$. Therefore, reparametrizations of imaginary time, $\tau\rightarrow\tau'(\tau)$, that are both invertible ($d\tau/d\tau'>0$) and consistent with the association rule: $\tau(-\tau')=-\tau(\tau')$, ($\tau(-T'/2)=-T/2$, $\tau(T'/2)=T/2$), leave S invariant.

The second property of action is that we can recover its value even if we know bounce only up to an τ-dependent invertible linear transformation $N(\tau)$, if $N(\tau)=I$ at $\tau=\pm T/2$ and $\tau=0$. Consider states $\psi_k(\tau)$ related to bounce $\phi_k(\tau)$ by means of:

$$\phi_k(\tau)=\sum_l N_{lk}(\tau)\psi_l(\tau). \tag{11}$$

Suppose that the overlaps $\langle\psi_k(-\tau)\mid\ \psi_l(\tau)\rangle$ are given by the matrix $M(\tau)$:

$$M_{kl}(\tau)=\langle\psi_k(-\tau)\mid\ \psi_l(\tau)\rangle, \tag{12}$$

so that $M(-\tau)=M(\tau)^+$. The condition $\langle\phi_k(-\tau)\mid\phi_l(\tau)\rangle=\delta_{kl}$ means that $N^+(-\tau)M(\tau)N(\tau)=I$ which leads to: $M^{-1}(\tau)=N(\tau)N^+(-\tau)$. Calculate action in terms of states $\psi_k(\tau)$. The integrand is:

$$\sum_{kl}M^{-1}_{lk}(\tau)\langle\psi_k(-\tau)\mid\partial_\tau\psi_l(\tau)\rangle+\sum_{il}N^{-1}_{il}(\tau)(\partial_\tau N_{li}(\tau)). \tag{13}$$

The second term is just: $TrN^{-1}\partial_\tau N=\partial_\tau(\ln\det N)$. From Eq. (6) one obtains:

$$S/\hbar=2\Re\int_{-T/2}^{0}d\tau\sum_{kl}M^{-1}_{lk}(\tau)\langle\psi_k(-\tau)\mid\partial_\tau\psi_l(\tau)\rangle, \tag{14}$$

where the omitted residual term, $\Re\int_{-T/2}^{0}d\tau\partial_\tau\ln\det N(\tau)$ is identically zero.

If one represents bounce in terms of some orthonormal HF orbitals $\psi_k(\tau)$, then HF determinants $\mid\Psi(\tau)\rangle$, built out of $\psi_k(\tau)$, are related to bounce determinant states $\mid\Phi(\tau)\rangle$ by: $\mid\Phi(\tau)\rangle=\det N(\tau)\mid\Psi(\tau)\rangle$, so that $\langle\Psi(-\tau)\mid\Psi(\tau)\rangle=\det M(\tau)$ and $\mathcal{H}=\langle\Phi(-\tau)\mid\hat{H}\mid\Phi(\tau)\rangle=\langle\Psi(-\tau)\mid\hat{H}\mid\Psi(\tau)\rangle/\langle\Psi(-\tau)\mid\Psi(\tau)\rangle$. Therefore, energy overlap $\mathcal{H}$ and action do not involve $N(\tau)$ since

$$\mathcal{H}=\sum_i\langle\psi_i(-\tau)\mid\hat{t}\mid\psi'_i(\tau)\rangle+\frac{1}{2}\sum_{i,j}\langle\psi_i(-\tau)\psi_j(-\tau)\mid\hat{v}\mid\psi'_i(\tau)\psi'_j(\tau)-\psi'_j(\tau)\psi'_i(\tau)\rangle, \tag{15}$$

where the states $\psi'(\tau)$ are related to $\psi(\tau)$ via: $\psi'_i(\tau)=\sum_k M^{-1}_{ki}(\tau)\psi_k(\tau)$. Since the density $\rho(\tau)=\sum_i\psi^*_i(-\tau)\psi'_i(\tau)$, the same holds for s.p. Hamiltonian $\hat{h}$ if it depends only on density. However, Eq. (3) do involve $N(\tau)$:

$$\partial_\tau\psi_k+\sum_l\left[\partial_\tau NN^{-1}\right]_{lk}\psi_l+\hat{h}\psi_k-\sum_l\left[\sum_m N^{-1}_{mk}\epsilon_m N_{lm}\right]\psi_l=0. \tag{16}$$

5. The question is whether Eq. (14) provides a proper upper bound for instanton action when applied for trial sets of orthonormal s.p. states $\psi_{1i}(\tau)$, $\psi_{2j}(\tau)$ on $-T/2<\tau<0$, with $\psi_k(\tau)=\psi_{1k}(\tau)$ and $\psi_k(-\tau)=\psi_{2k}(-\tau)$, $\mathcal{H}=E_{gs}$ and the overlap matrix $M_{kl}(\tau)=\langle\psi_{2k}(\tau)\mid\psi_{1l}(\tau)\rangle$ for $\tau<0$, and $M(\tau)=M(-\tau)^+$ for $\tau>0$. The answer is in negative, although the action so calculated, under reasonable conditions, will usually show a minimum.

As an example, consider both sets labeled by a collective coordinate q (e.g. quadrupole moment), $q_1(\tau)$ and $q_2(\tau)$, $\tau<0$ (not necessarily adiabatic). Through the barrier, $q_2(\tau)$ must be different from $q_1(\tau)$ to make energy overlaps $\langle\Psi(q_2(\tau))\mid\hat{H}\mid\Psi(q_1(\tau))\rangle/\langle\Psi(q_2(\tau))\mid\Psi(q_1(\tau))\rangle$ equal to E_{gs}. For a path: $\psi_k(\tau)=\psi_k(q_1(\tau))$ for $\tau<0$, and $\psi_k(q_2(-\tau))$ for $\tau>0$ one obtains the integrand $Tr(M(q_2,q_1)^{-1}\partial_{q_1}M(q_2,q_1))$ and therefore:

$$S=2\hbar\Re\int_{q(-T/2)}^{q(0)}dq_1\frac{\partial\ln\det M(q_2,q_1)}{\partial q_1} \tag{17}$$

with $M_{kl}(q_2,q_1)=\langle\psi_k(q_2(-\tau))\mid\psi_l(q_1(\tau))\rangle$. When the labeling of states involves more collective coordinates denoted as $\vec{Q}$, the previous formula modifies to:

$$S=2\hbar\Re\int_{\vec{Q}_1(-T/2)}^{\vec{Q}_1(0)}d\vec{Q}_1\cdot\nabla_{\vec{Q}_1}\ln\det M(\vec{Q}_2,\vec{Q}_1). \tag{18}$$

This can serve to explain the sign of S: As shown by the bounce equations (3), for $\tau < 0$, on the way from the g.s. through the barrier, the deformation $\vec{Q}_2$ of the state $\Psi(-\tau)$ drags deformation $\vec{Q}_1$ of $\Psi(\tau)$; thus $\vec{Q}_1$ lags behind $\vec{Q}_2$, and *vice versa* on the way back. Therefore, increasing Q_{1i} along the fission path while keeping fixed Q_{2j} *decreases* separation between $\vec{Q}_2$ and $\vec{Q}_1$, and thus increases the overlap $\det M(\vec{Q}_2, \vec{Q}_1)$. Hence, the integrand in (18), and thus action S, is positive.

In the above reasoning we used the property of the bounce equation. While using a variational principle, one might exchange the states Ψ_1 and Ψ_2, and then, by the previous reasoning, negative action would follow. One might try $\mid S \mid$ as an answer in such a case, and there are cases, when this way of proceeding defines a minimum. However, it is clear that some additional conditions are necessary.

With the condition $q_2 > q_1$, the formula (17) may be shown similar (modulo approximations) to one of the standard treatments of quantum tunneling. Namely, one may expand the integrand in Eq. (17) with respect to the quadrupole moment difference $s = q_2(\tau) - q_1(\tau)$ around the midpoint $\bar{q} = (q_1 + q_2)/2$. In the Gaussian overlap approximation (GOA), $\ln \det M(q_2, q_1) \approx -\gamma(\bar{q}) s^2/2$ and after disregarding quadratic and higher order terms in the integrand, one obtains:

$$S \approx 2\hbar \int_{q(-T/2)}^{q(0)} dq_1 \gamma(\bar{q})(q_2 - q_1), \tag{19}$$

where, as discussed above, $q_2(q_1) > q_1$, and $\gamma(\bar{q}) = \sum_k \langle \partial_q \psi_k \mid \partial_q \psi_k \rangle - \sum_{kl} \langle \partial_q \psi_k \mid \psi_l \rangle \langle \psi_l \mid \partial_q \psi_k \rangle$. The integration variable $dq_1 = d\bar{q} - ds/2$ may be changed to $d\bar{q}$, as the integral $sds = d(s^2)/2$ between endpoints with $s = 0$ vanishes. The quadrupole moment splitting may be calculated from the constraint on energy overlap: $E_{gs} = \mathcal{H}[q_2, q_1] \approx \mathcal{H}[\bar{q}, \bar{q}] - s^2(\mathcal{H}_{xy} - \mathcal{H}_{xx})/4$, where we used a symbolic notation for derivatives of $\mathcal{H}$ (cf. [8], where the explicit formulas for those are given). Since the diagonal value of the energy overlap is just "potential energy" $V(\bar{q})$ in the standard approach, one obtains:

$$S \approx 2\hbar \int_{q(-T/2)}^{q(0)} d\bar{q} \sqrt{2\left(V(\bar{q}) - E_{gs}\right)\left(\frac{2\gamma(\bar{q})^2}{\mathcal{H}_{xy} - \mathcal{H}_{xx}}\right)}, \tag{20}$$

where the quantity in the second parenthesis is the GOA mass parameter (cf. [8]).

6. The reparametrized bounce, $\{\phi_k(\tau(\tau'))\}$ ceases to solve the equations (3). Instead, it solves a different one (we omit terms assuring periodicity, which are immaterial for the argument):

$$\hbar \frac{\partial \phi_k}{\partial \tau'}(\tau') + \left(\frac{d\tau}{d\tau'}\right) \hat{h}(\tau(\tau'))\phi_k(\tau') = 0, \tag{21}$$

where, $d\tau/d\tau'(-\tau') = d\tau/d\tau'(\tau')$ as a consequence of properties of $\tau(\tau')$. This equation can be presented as:

$$\frac{\delta S}{\delta \phi_k^*(-\tau')} - \lambda(\tau') \frac{\delta \mathcal{H}}{\delta \phi_k^*(-\tau')} = 0, \tag{22}$$

and looks like the condition for the vanishing first variation of action S under the constraint of constant $\mathcal{H}$, with the Lagrange multipliers $\lambda(\tau') = -\frac{d\tau}{d\tau'}$.

Indeed, the Eq. (22) with a real $\mathcal{H}$ imposes the property $\lambda(-\tau') = \lambda(\tau')$, as for a derivative $d\tau/d\tau'$ of some reparametrization $\tau(\tau')$. The condition of the constant sign of $\lambda(\tau')$ also follows from Eq. (22). The solutions with $\lambda(\tau') < 0$ are just instantons. As the instantons inverted in imaginary time, satisfy the equation:

$$-\hbar \frac{\partial}{\partial \tau'} \phi_k(-\tau') - \lambda(-\tau') \hat{h}(-\tau') \phi_k(-\tau') = 0. \tag{23}$$

they also correspond to solutions of Eq. (22), but with positive $\lambda(\tau')$. As can be seen from Eq. (6), the interchange of $\phi_k(\tau)$ with $\phi_k(-\tau)$ inverts the sign of S. Thus, the principle of the minimization of S requires additional conditions.

To make the bounce action minimal, one must satisfy half of the instanton equations, e.g. those for $\tau < 0$. As the structure of Eq. (22) suggests, $\phi(\tau)$ and $-\phi_k^*(-\tau)$ are conjugate variables, so one should find such $\phi_k(-\tau)$ which drag $\phi_k(\tau)$ ($\tau < 0$) according to these equations, producing correct $\partial_\tau \phi_k(\tau)$. This is in full analogy with mechanics, where one minimizes $\int \sum_i p_i dq_i$ under the condition of constant energy *and provided* that canonical relations $\dot{q}_i = \partial \mathcal{H}/\partial p_i$ are satisfied on each path.

For constant s.p. overlaps, action is fixed by the integral over $\tau < 0$. It will be minimal for $\phi_k(-\tau)$ also fulfilling the equations. Since the equations are non-linear, one cannot easily substitute velocities for momenta, as in the mechanical case.

Thus, to find instantons, one has to minimize action S over fission paths which fulfill bounce boundary conditions, velocity-momentum conditions, and the energy condition $\mathcal{H} = E_{gs}$. Since the properties of solutions to (21) are not assured for trial paths, the condition of constant s.p. overlaps should be imposed on them independently.

Perhaps another representation of the instanton better illustrates velocity-momentum relation. One can define: $\phi_k(\tau) = A_k(\tau) - B_k(\tau)$, $\phi_k(-\tau) = A_k(\tau) + B_k(\tau)$. It follows that $A_k(-\tau) = A_k(\tau)$ and $B_k(-\tau) = -B_k(\tau)$. Due to the boundary conditions, $A_k(\pm T/2) = \psi_k^{HF}$, $A_k(0) = \phi_k(0)$, $B_k(\pm T/2) = B_k(0) = 0$. Thus A_k define some average tunneling states (coordinates), while B_k, the differences between instanton bra and kets, are the driving fields for A_k (momenta). These two sets of states fulfill the system of equations:

$$\hbar \frac{\partial}{\partial \tau} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = - \begin{pmatrix} i\hat{h}_I & , \ \epsilon_k - \hat{h}_R \\ \epsilon_k - \hat{h}_R \ , & i\hat{h}_I \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix}, \tag{24}$$

where we used decomposition of $\hat{h}(\tau) = \hat{h}_R + i\hat{h}_I$ with hermitean $\hat{h}_R(-\tau) = \hat{h}_R(\tau)$ and $\hat{h}_I(-\tau) = -\hat{h}_I(\tau)$. The conserved overlaps in terms of the amplitudes A_k and B_k read: $\langle A_k \mid A_l \rangle - \langle B_k \mid B_l \rangle = \delta_{kl}$, and $\langle A_k \mid B_l \rangle - \langle B_k \mid A_l \rangle = 0$. The density is: $\rho = \sum_k (\mid A_k \mid^2 - \mid B_k \mid^2 - 2i\Im(A_k^* B_k))$. Due to the symmetry properties of the amplitudes, action reads

$$S/\hbar = 2\Re \int_{-T/2}^{T/2} d\tau \sum_k \left\langle B_k \middle| \frac{\partial A_k}{\partial \tau} \right\rangle. \tag{25}$$

The first set of the equations (24) should be fulfilled on trial trajectories in order to assure a minimum of action for bounce. For the cases when $\hat{h}_I = 0$, i.e. for the hermitean s.p. Hamiltonian, this gives a formula deceptively similar to the cranking expression:

$$S = 2\hbar^2 \int_{-T/2}^{T/2} d\tau \sum_k \left\langle \frac{\partial A_k}{\partial \tau} \middle| \frac{1}{\hat{h}(\tau) - \epsilon_k} \middle| \frac{\partial A_k}{\partial \tau} \right\rangle. \tag{26}$$

However, the self-consistent dependence of $\hat{h}$ on B_k makes all the difference. It also makes the enforcement of velocity-momentum conditions on trial paths difficult.

Conclusions:

The search for a mean-field instanton and associated decay exponent is formulated as a variational problem in a space of HF states which provide trial fission paths. The specific nature of imaginary-time mean-field equations requires that each path consist of two, necessarily different, branches. For each mean-field state of one branch, there is an associated state of the second branch and together they serve as bra and ket in the calculation of observables.

The formulas (6,18) express action for an instanton in terms of its HF representation. The minimization of action under the constraint of constant energy overlap requires additional conditions (momentum-velocity relations). Their solution must be simplified to make a variational approach feasible.

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