Pair breaking in nuclear fission

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Abstract

A simple model is proposed to estimate the probability of breaking the pairing between nucleons during the scission phase of nuclear fission. The model reduces the pairing dynamics to a three-dimensional time-dependent Hamiltonian matrix. One of its matrix elements is assumed to vary linearly with time, similar to the Landau-Zener treatment of level crossings. The time-dependent Hamiltonian equation is solved to calculate the dependence of pair-breaking probability on the scission duration time t_s and other physical parameters. The results suggest that the transition dynamics is closer to the adiabatic limit than to the sudden limit for scission durations $t_s > 700$ fm/c.

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I. INTRODUCTION

The odd-even staggering of fission fragment charge Z or mass number A is poorly understood. Adiabatic dynamics of a fissioning even-even nuclei in its ground state would yield even-even fragments only. But in fact the production of odd-Z fragments is often nearly as likely as odd-Z fragments [1].In dynamical theories of fission there are two mechanisms to break nucleon pairs[2]. The first is the excitation of quasiparticles in the descent of the system from the barrier to the scission point. This is often described by a phenomenological coupling of the collective motion to a heat bath of internal excitations. The other mechanism involves the quantum dynamics at the scission point. If the scission occurs quickly, nucleons will populate the individual fragments according to the probability densities of the orbital wave functions in the pre-scission nucleus. This is the sudden limit. It is often invoked in calculating properties of fission fragments[5–7]. On the other hand, if the scission is a slow process the adiabatic extreme is more appropriate. Here the orbital containing the paired nucleons in the pre-scission nucleus will transform into an orbital residing entirely in one fragment or the other [8].

A model is proposed here to provide a framework for estimating how the speed of the scission affects the probability that nucleons paired before scission end up in different fragments. There are two distinct issues to be dealt with. The first concerns the many-particle physics associated with pairing collectivity as was analyzed for example in Refs. [7, 9, 10]. That modeling requires understanding the role of a condensate and of finite occupation probabilities in excited configurations[11, 12]. These aspects are beyond the scope of this study. The second issue, which is the focus here, is the evolution of a typical orbital pair under the time-dependent dynamics. As discussed below, much of the dynamics is already incorporated in the time-dependent Hartree-Fock-Bogoliubov (HFB) approximation, for example, as applied in Ref. [13]. However, a real understanding of the pair-breaking dynamics is crucial for building calculational frameworks, including versions of includes approximations mean-field theory such as the time-dependent generator coordinate method, as theories that go beyond the mean field.

[1] See Refs. [1, 2] for examples of experimental measurements.
[2] This excludes purely statistical models, eg. Ref. [3, 4].

II. HAMILTONIAN

Near the scission point, the deeply bound orbitals are localized on one side or the other, except for rare degeneracies. Orbitals near the Fermi level may have significant probabilities on both sides of the neck, and their time evolution is the object of this study. I assume that such orbitals can be expressed as a linear combination of single-particle wave functions localized on the left and right, denoted by $\phi_{\ell K}$ and $\phi_{r,K}$ respectively. Here K is the usual azimuthal angular momentum in an axially symmetric single-particle Hamiltonian. The orbitals are assumed to maintain their Kramers' degeneracy during the fission, so the orbital space includes both K and $-K$ wave functions, denoted $\uparrow$ and $\downarrow$ below. The Hamiltonian matrix will be applied in the basis of two-particle configurations given by

$$\vec{\psi} = \begin{pmatrix} \psi_1 \\ \psi_{bp} \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \phi_{\ell\uparrow}\phi_{\ell\downarrow} \\ \frac{1}{\sqrt{2}}\left(\phi_{\ell\uparrow}\phi_{r\downarrow} + \phi_{r\uparrow}\phi_{\ell\downarrow}\right) \\ \phi_{r\uparrow}\phi_{r\downarrow} \end{pmatrix}. \tag{1}$$

Note that the full two-particle space is 6-dimensional; the truncated basis omits a subspace that has no coupling to the paired configurations. The single-particle Hamiltonian H_{sp} is parametrized as

$$\langle xK|H_{sp}|x'K'\rangle = \left(\varepsilon_x\delta_{xx'} + v_{\ell r}(\delta_{x\ell}\delta_{x'r} + \delta_{xr}\delta_{x',\ell})\right)\delta_{KK'}. \tag{2}$$

The Hamiltonian also includes the pairing component of the two-particle interaction. The nonzero matrix elements are taken to be the diagonal ones

$$\langle\psi_i|H_p]\psi_i\rangle = -G \ \text{ for } i = 1, 2. \tag{3}$$

Here G is the effective strength of the interaction. The off-diagonal pairing matrix element $\langle\psi_1|H_p]\psi_4\rangle$ is neglected: it is much smaller than G due to the small overlap between ℓ and r orbitals. The resulting Hamiltonian in the three-dimensional space is

$$H^{(3)}_{eff} = H_{sp} + H_p = \begin{pmatrix} -\varepsilon_{\ell r} - G & \sqrt{2}v_{\ell r} & 0 \\ \sqrt{2}v_{\ell r} & 0 & \sqrt{2}v_{\ell r} \\ 0 & \sqrt{2}v_{\ell r} & \varepsilon_{\ell r} - G \end{pmatrix} \tag{4}$$

where $\varepsilon_{\ell r} = \varepsilon_r - \varepsilon_\ell$ and an overall constant has been omitted. As an aside, note that the dynamics can be further simplified to a two-dimensional space if one assumes that the

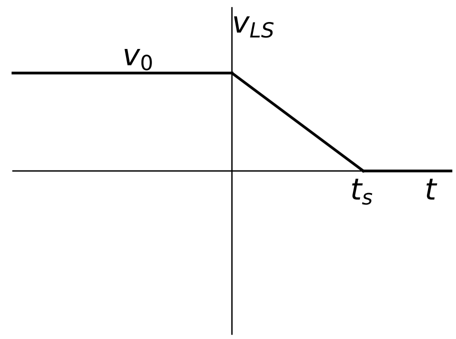

FIG. 1: Time dependence of $v_{\ell r}$

diagonal energies are completely dominated by either $\varepsilon_{\ell r}$ or G. Without the interaction term G the dynamics is pure mean-field, resulting in identical amplitudes for K and $-K$ orbitals[3]. Then the equation of motion can be expressed in the two-dimensional subspace of either K. On the other hand, if the single-particle energy difference can be neglected, ψ_1 and ψ_4 will have identical amplitudes and $H^{(3)}$ in Eq. (4) can be reduced to a two-dimensional Hamiltonian in the space $[(\psi_1+\psi_4),(\psi_2+\psi_3)]/\sqrt{2}$.

The physical observable to be calculated is the probability of the broken pair configurations,

$$P_b = |\psi_{bp}|^2. \tag{5}$$

The parameters G and $\varepsilon_{\ell r}$ are assumed to be constant while the single-particle term $v_{\ell r}$ varies with time. It starts at some nonzero value v_0 before scission and diminishes to zero after the nascent fragments separate. A simple way to parametrize it assumes a linear dependence,

$$v_{\ell r}(t) = v_0\,(1 - t/t_s)\,, \quad 0 < t < t_s \tag{6}$$

as illustrated in Fig. 1. Here t_s is the duration of the scission dynamics starting from an adiabatically generated configuration and ending when the two nascent fission fragments are no longer in contact. Thus the model has four parameters, $\varepsilon_{\ell r}, G, v_0$, and t_s.

The calculations of pair breaking are carried out as follows. First, the starting wave function $\vec{\psi}(0)$ is taken as the ground state of the effective Hamiltonian with the given parameters

[3] A much more detailed model in the same spirit was proposed in Ref. [14].

$G, \varepsilon_{\ell r}$, and v_0. The initial broken-pair probability is $P_{b0} = |\psi_{bp}(0)|^2$. The wave function is then evolved by the time-dependent Hamiltonian equation

$$i\hbar \frac{d}{dt}\vec{\psi}(t) = H^{(3)}\vec{\psi}(t). \tag{7}$$

At $t = t_s$ the coupling between paired and unpaired components vanishes and P_b reaches its final value P_{bf}. This will be the quantity of interest in the present study. Crude estimates of the parameters are given in the Section III below. Section IV following presents the resulting probabilities P_{b0} and P_{bf} for a variety of parameter sets.

III. PARAMETER SPECIFICATION

A. The parameter G

. Eq. (3) for the pairing matrix elements implicitly assumes that a pairing condensate is weak or absent. This is a reasonable assumption at scission, because the internal excitation energy of the pre-scission nucleus is likely to quench any BCS condensate. This was also found to be the case in time-dependent HFB calculations [13]. Given that the system is in the normal phase of a Fermi gas, the interaction would be some residual two-body interaction in a more realistic Hamiltonian. A typical parameterization appropriate for BCS calculations in a single major shell is $G = 25/A$ MeV. Numerically, that interaction strength is $G \approx 0.15$ MeV at the masses A of the fission fragments. However, the effective strength might be higher due to the many-body enhancement of pairing energies; in the presence of a ground-state condensate it approaches the pairing gap Δ often parametrized as $\Delta = 12/A^{1/3}$ MeV.

B. The parameter t_s

Even if one had a precise definition of its starting and ending points, there would still be much uncertainty about the duration of the scission event. One set of calculations carried out in the time-dependent Hartree-Fock-Bogoliubov (HFB) framework found scission times in the range of 1000 -14000 fm/c [13]. Other calculations based on the time-dependent HF or HF-BCS approximations for the nucleus ^{264}Fm report smaller durations, 1.6×10^{-21} s ≈ 500 fm/c in Ref. [15] and 600 - 1600 fm/c in Ref. [16]. That particular nuclide may fission into two doubly magic ^{132}Sn nuclei. This makes the conditions for a fast scission very favorable; the t_s for other actinides are likely to be much higher.

C. The parameter $\varepsilon_{\ell r}$

When the pre-fission nucleus finally undergoes scission, each HFB-paired orbital divides into two, one on the right-hand fragment and the other on the left-hand fragment. Their single-particle energies have no relation to each other in asymmetric fission and thus can only be treated probabilisticly. Linking the orbital in one nucleus to the closest orbital of the same K in the other nucleus leads to a distribution uniform in $\varepsilon_{\ell r}$ extending from $\varepsilon_{\ell r} = 0$ to $\Delta\varepsilon/2$, where $\Delta\varepsilon$ is the energy spacing of orbitals of a particular K value in one of the fragments. Following this reasoning, the average is $\langle \varepsilon_{\ell r} \rangle \approx \Delta\varepsilon/4$. The $K = 1/2$ orbitals will have the strongest connections to the two nuclei. Some indication of $\Delta\varepsilon$ can be extracted from Fig. 5 of Ref. [8]. The upper panel shows 6 neutron orbitals of the combined system in an energy window of 8 MeV centered at the Fermi energy. For a given ϕ_ℓ and ϕ_r there are two orbitals in the combined system. This leads to the estimate $\Delta\varepsilon = 8 * 2/6 = 2.7$ MeV for the $K = 1/2$ orbitals in a daughter nucleus and $\varepsilon_{\ell r} = 2.7/4 = 0.7$ MeV for the average single-particle energy differences. This value will be used in the numerical calculations below.

D. The parameter v_0

The initial coupling between ℓ and r orbitals v_0 is not a quantity that can be easily extracted from published time-dependent mean-field calculations. For one thing, the initial conditions are ambiguous without a precise definition of the starting point for scission. However, as will be seen below, at least one aspect of pair breaking is rather insensitive to v_0. If v_0 is large, the wave function does not change much in the early stage of scission. It is only when $v_{\ell r}(t)$ becomes comparable to the other energy parameters that non-adiabatic effects become important. I will consider range of values $v_0 = 0.25-1.0$ MeV in the numerical calculations below.

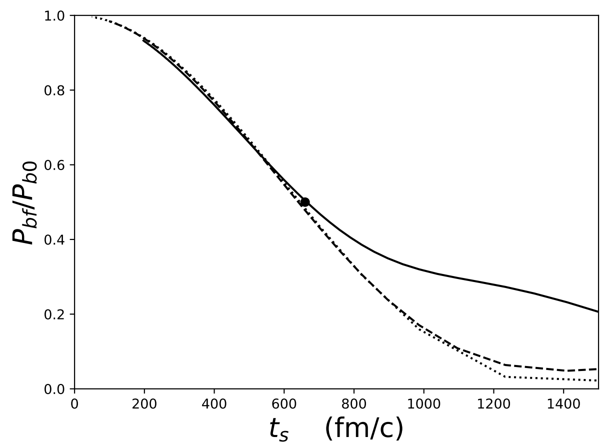

FIG. 2: Probability of pair breaking P_b in final state for the three-dimensional model, plotted as a function of the scission duration time t_s. The three curves show P_b for $v_0 = 0.25, 0.5$, and 1.0 MeV for the dotted, dashed and solid lines respectively. The other parameters in the Hamiltonian are $\varepsilon_{\ell r} = 0.7$ MeV and $G = 0.15$ MeV.

$\varepsilon_{\ell r}$	G	v_0	P_{b0}	t_s
0.7	0.15	1.0	0.425	665
”	”	0.5	0.296	640
”	”	0.25	0.131	645
0	0.85	1.0	0.396	667
0.85	0.0	1.0	0.424	621
1.7	0.0	2.0	0.424	310

TABLE I: Initial pair-breaking probability and scission duration times for a variety of Hamiltonian parameters. The parameters $\varepsilon_{\ell r}$, G, and v_0 are in units of MeV; the parameter t_s is in units of fm/c.

IV. NUMERICAL CALCULATIONS

The numerical results solving Eq. (7) for a variety of parameters are presented in Fig. 2 and Table I. In the Figure the parameters $\varepsilon_{\ell r}$ and G are taken at their default values given in Sec. III B. The three curves show the suppression factor P_{bf}/P_{b0} for three values of v_0, plotted as a function of t_s. One sees that the P_{bf} approaches the sudden approximation for small t_s and the adiabatic limit at large t_s. The filled circle marks the point on the solid curve where the pairing-breaking probability is halfway between the adiabatic and sudden limits. It is located at $t_s = 665$ fm/c. The dividing point between dynamics close to adiabatic and dynamics close to the sudden approximation may be taken the point where $P_{bf} = P_{b0}/2$. It is marked by a solid circle on the graph for $v_0 = 1.0$ MeV, located at $t_s = 660$ fm/c. Remarkably, the half-adiabatic point is at nearly the same t_s for the other curves as well. Thus, a least one aspect of the pair-breaking dynamics is weakly dependent on v_0.

In Table I, the top three lines report the numerical values of P_{b0} and t_s at the half-adiabatic point for the three cases shown in Fig. I. The next two lines show the variation with respect to $\varepsilon_{\ell r}$ and G, holding their sum fixed to the same value as in the first line of the Table. One sees that the results are not much different. This shows that the dependence on $\varepsilon_{\ell r}$ and G is mainly in the combination $\varepsilon_{\ell r} + G$. The bottom line shows a trivial parameter change, namely doubling all the energy parameters from the previous line. Here one sees that t_s is decreased by a factor of two, as required from dimensional analysis.

In conclusion, I find that the main determinant of the non-adiabaticity of the scission dynamics (as defined by the half-adiabatic duration time) is the energy difference between the paired state ψ_1 and the broken-pair state ψ_b. This is not surprising from a qualitative standpoint; the model presents a way to make that statement quantitative.

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