Correlated fission fragment angular momenta

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Abstract. Nuclear fission produces fragments whose spins are coupled to each other as well as to the relative fragment motion due to angular momentum conservation. Statistical ensembles of such spins can readily be obtained by either direct microcanonical sampling or by sampling of the associated normal modes of rotation. The spin-spin opening angle distribution is illustrated for both 3D and 2D spin scenarios and it is demonstrated how recent calculations with various models can be well reproduced by the statistical results under different assumptions about the scission geometry.

1 Introduction

There is currently considerable interest in the correlations between the angular momenta of fission fragments. These are interesting because they reflect the microscopic mechanisms acting during the fission process. However, a number of mutually contradictory predictions have been made [1–3], generating some confusion. We present here a simple statistical framework within which such widely different results can emerge when the coupled spins are sampled under different assumptions. More details can be found in Ref. [4].

2 Framework

The treatment assumes that the two fragment spins, $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$, and the angular momentum associated with their relative motion, $\boldsymbol{S}_0 = \boldsymbol{R} \times \boldsymbol{P}$ form a statistical ensemble constrained by the conservation of the total angular momentum (assumed to vanish), $\boldsymbol{S}_0 + \boldsymbol{S}_1 + \boldsymbol{S}_2 = \boldsymbol{0}$. Thus, with regard to the angular momenta, the system forms a microcanonical ensemble. Because we shall here focus on the directional correlations, the distribution of the total energy E is immaterial and we shall assume it to be canonical, $P(E) \sim \exp(-E/T)$, where the particular value of the temperature T is arbitrary. The sampling of the fragment spins is illustrated by the expression for the associated phase space volume,

$$\Omega_T = \prod_{i=0}^{2} \left[\int d^D \boldsymbol{S}_i \, \mathrm{e}^{-S_i^2/2\mathcal{I}_i T} \right] \delta^{(D)}\left(\sum_{i=0}^{2} \boldsymbol{S}_i \right) = \left(\frac{\mathcal{I}_0 \mathcal{I}_1 \mathcal{I}_2}{\mathcal{I}_0 + \mathcal{I}_1 + \mathcal{I}_2} \right)^{\frac{1}{2}D} [2\pi T]^D \,, \qquad (1)$$

where $D = 2, 3$ is the dimensionality of the spins. The moments of inertia of the fragments are taken as those of rigid spheres, $\mathcal{I}_\mathrm{f} = \frac{2}{5} M_\mathrm{f} R_\mathrm{f}^2$, where M_f are the fragment masses, and $\mathcal{I}_0 = \mu R^2$ for the relative motion, with $\mu = M_1 M_2/(M_1 + M_2)$ being the reduced mass.

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One method for carrying out the constrained sampling consists in first sampling the energy E from its canonical distribution and then sampling the various angular momenta from the microcanonical ensemble characterized by that energy and the (vanishing) total angular momentum (see Ref. [4] for details).

Another method, described below, diagonalizes the problem and carries out the sampling in terms of the normal modes of rotation. These are obtained by bringing the rotational energy onto diagonal form,

$$E = \frac{S_1^2}{2\mathcal{I}_1} + \frac{S_2^2}{2\mathcal{I}_2} + \frac{|\boldsymbol{S}_1 + \boldsymbol{S}_2|^2}{2\mathcal{I}_0} = \frac{s_+^2}{2\mathcal{I}_+} + \frac{s_-^2}{2\mathcal{I}_-}, \tag{2}$$

where the moments of inertia of the normal modes are given by $\mathcal{I}_+^{-1} = [\mathcal{I}_1 + \mathcal{I}_2]^{-1} + \mathcal{I}_0^{-1}$ and $\mathcal{I}_-^{-1} = \mathcal{I}_1^{-1} + \mathcal{I}_2^{-1}$ [5]. The conservation of angular momentum is built into the normal modes $\boldsymbol{s}_\pm$, each of which carries no total angular momentum. The normal modes $\boldsymbol{s}_\pm$ may be sampled independently from the respective Boltzmann distributions, $P_\pm(\boldsymbol{s}_\pm) \sim \exp(-s_\pm^2/2\mathcal{I}_\pm T)$, and the individual fragment spins can then readily be constructed subsequently [4],

$$\boldsymbol{S}_1 = [\mathcal{I}_1/(\mathcal{I}_1 + \mathcal{I}_2)]\, \boldsymbol{s}_+ + \boldsymbol{s}_- \,, \quad \boldsymbol{S}_2 = [\mathcal{I}_2/(\mathcal{I}_1 + \mathcal{I}_2)]\, \boldsymbol{s}_+ - \boldsymbol{s}_- \,, \tag{3}$$

with the orbital angular momentum following as $\boldsymbol{S}_0 = -\boldsymbol{S}_1 - \boldsymbol{S}_2 = -\boldsymbol{s}_+$. The mode sampling method has the advantage that different temperatures can be employed for different modes, thus making it possible to control their relative presence, as was recently exploited [5].

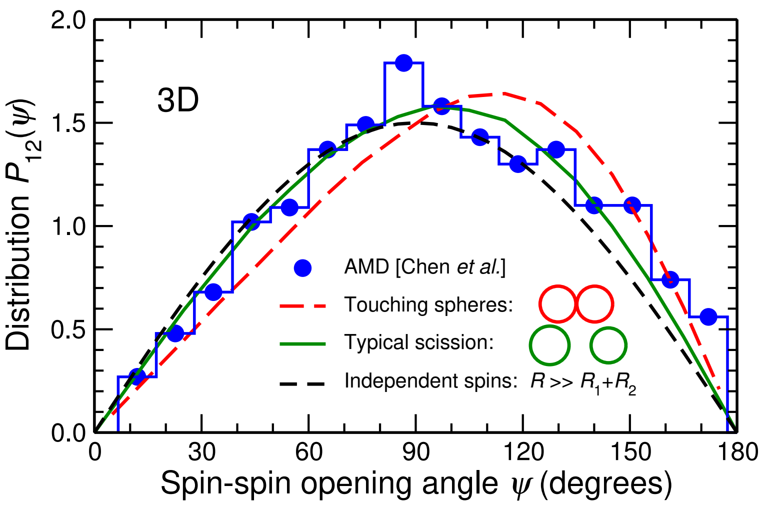

Figure 1. The statistical distribution of the fragment spin opening angle ψ for 3D spins in various scenarios: *Touching spheres:* A schematic reference scenario of two touching spheres of equal size in which case the relative sizes of the moments of inertia are $\mathcal{I}_1 : \mathcal{I}_2 : \mathcal{I}_0 = 1 : 1 : 5$; *Typical scission:* A realistic scenario in which case the moments of inertia have the ratios 1 : 1 : 17; and *Independent spins:* The limiting scenario for large $\mathcal{I}_0$ where the angular-momentum constraint is ineffective and the two fragment spins become independent. Also shown are the results obtained with Antisymmetrized Molecular Dynamics for fission of (excited) ^{252}Cf (from Ref. [3]).

3 Spin-spin opening angle

We focus here on one particular angular-momentum related observable, namely the opening angle between the two fragment spins, ψ, which in each sampled event can be otained from $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 = S_1 S_2 \cos\psi$. Figure 1 illustrates the distribution $P(\psi)$ for various reference scenerios for three-dimensional spins, $D = 3$.

If the two spins were independent, as they become in the limit of very elongated scission configurations where $\mathcal{I}_0 \gg \mathcal{I}_\mathrm{f}$, the distribution is symmetric around 90°, $P(\psi) \sim \sin\psi$. For more realistic scenarios, the requirement of angular momentum conservation skews the distribution towards larger angles. An instructive (but unreaslitic) scenario is that of equal touching spheres, for which $\mathcal{I}_\mathrm{f} : \mathcal{I}_0 = 1 : 5$, in which case $P(\psi)$ peaks near $\psi \approx 115°$. For realistic scission configurations, the separation between the two fragment centers exceeds the sum of their radii by several fm and $\mathcal{I}_0$ is nearly 20 times as large as $\mathcal{I}_\mathrm{f}$ [4]; consequently, the effects of conservation are not expected to be large.

4 Antisymmetrized molecular dynamics

At a recent workshop in Seattle, results for $P(\psi)$ obtained with Antisymmetrized Molecular Dynamics (AMD) were presented [3] and they have been included in Fig. 1.

AMD represents the state of the system by a Slater determinant of Gaussian wave packets whose centroids are propagated by classical equations of motion with the potential energy having been augmented by the repulsive effect of the antisymmetrization. This implies a short mean free path for the individual centroids and a rapid local equilibration might therefore be expected. This appears to be indeed borne out by the AMD results for the distribution of the spin-spin opening angle which is consistent with the 3D equilibrium form in Fig. 1 corresponding to realistic scission shapes.

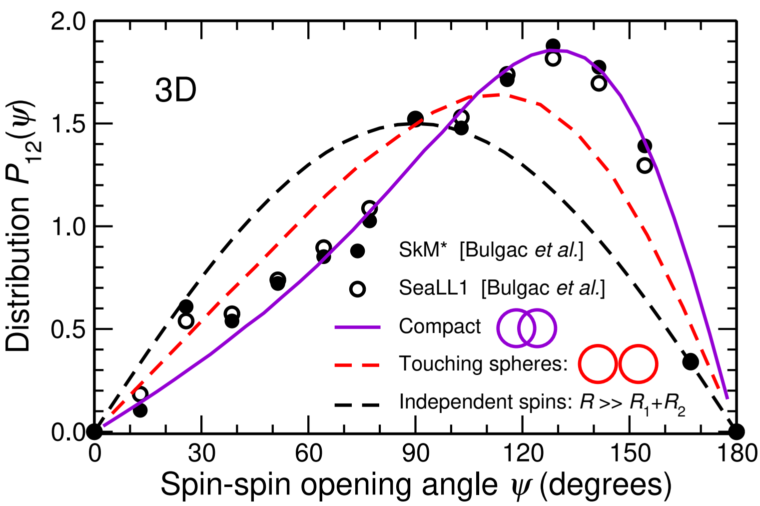

Figure 2. The opening-angle distributions calculated by Bulgac *et al.* [2] with time-dependent density functional theory using either the SkM* or the SeaLL1 energy density functional are compared with the statistical distributions for 3D spins for *independent spins* and for *touching spheres*. Also shown is the distribution for a *compact* scenario where $\mathcal{I}_0 = \mathcal{I}_1 + \mathcal{I}_2$.

5 Time-dependent density functional theory

The spin-spin opening-angle distribution has also been calculated using time-dependent density functional theory [2], another self-consistent quantal model; these results are shown in Fig. 2. The calculations were carried out with both the SkM* or the SeaLL1 energy density functional and the two resulting distributions are rather similar.

These distributions are quite remarkable because they peak near $\approx 128^\circ$ which is beyond what is obtained for touching fragments. Nevertheless, a good reproduction of those distributions can be obtained within the present statistical framework by employing very compact scission configurations. As Fig. 2 shows, the calculated $P(\psi)$ can be well reproduced by 3D samplings that employ the ratios $\mathcal{I}_1:\mathcal{I}_2:\mathcal{I}_0 = 1:1:2$, corresponding to using $\mathcal{I}_0 = \mathcal{I}_1 + \mathcal{I}_2$. Such a value of $\mathcal{I}_0$ is only 40% of that for touching spheres, and about an order of magnitude below those for typical scission configurations, and it corresponds to the two fragments overlapping significantly, as indicated on the figure. As of yet, there is no explanation of this puzzling result.

6 FREYA simulations

The first calculations of $P(\psi)$ were made with the fission model FREYA which assumes that the fragment spins are perpendicular to the fission axis [1]. It was found that, apart from the restriction of being two-dimenional, the spins were nearly independent, in magnitude as well as direction [6, 7]. Accordingly, $P(\psi)$ exhibited only a small undulation away from constancy, as shown in Fig. 3.

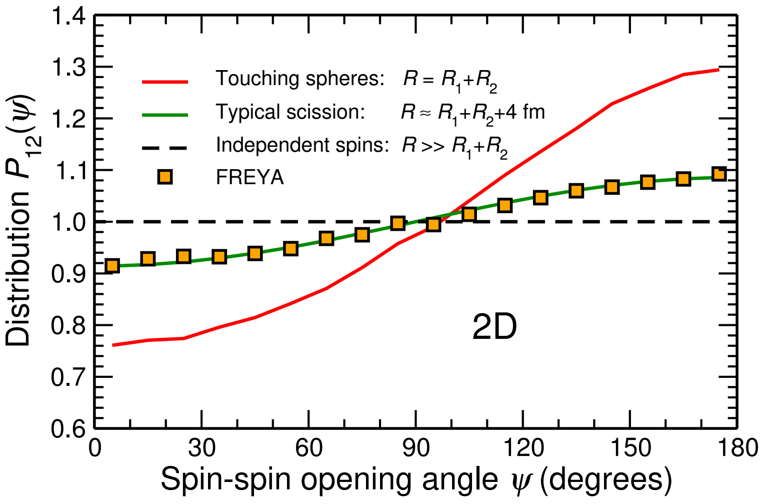

Figure 3. The statistical distribution of the fragment spin opening angle ψ_{12} for 2D spins in various scenarios: *Touching spheres:* A schematic reference scenario of two touching spheres of equal size in which case the relative sizes of the moments of inertia are $\mathcal{I}_1 : \mathcal{I}_2 : \mathcal{I}_0 = 1 : 1 : 5$; *Typical scission:* A realistic scenario in which case the moments of inertia have the ratios 1 : 1 : 17; and *Independent spins:* The limiting scenario for large $\mathcal{I}_0$ where the momentum constraint is ineffective and the two fragment spins become independent. Also shown is the distribution obtained with the fission event generator FREYA (from Ref. [6]).

In the reference scenario of totally independent spins, $\mathcal{I}_0/\mathcal{I}_\mathrm{f} \to \infty$, the directions of the fragment spin vectors are distributed uniformly in the perpendicular plane and it follows that the distribution of the opening angle ψ is constant, $P(\psi) = 1$.

When the coupling to the orbital motion is taken into account in the sampling, the two fragment spins have a slight preference for being directed oppositely, because that leads to a smaller orbital angular momentum, $S_0 = |S_1 - S_2|$, and is therefore energetically favored. The opening-angle distribution is typically well represented by the first-order Fourier approximation, $P(\psi) \approx 1 + f_1 \cos\psi$, and the deviation from uniformity is fairly small when realistic moments of inertia are used, $f_1 = -0.086$ [4].

As was the case for 3D spins, the touching-sphere scenario, with its considerably smaller $\mathcal{I}_0$, leads to larger deviations of $P(\psi)$ from the independent scenario, namely $f_1 = -0.264$, and the inclusion of the second-order Fourier term is required for an accurate representation, $P(\psi) \approx 1 + f_1 \cos\psi + f_2 \cos 2\psi$, with $f_2 = 0.028$ [4].

The current fission model FREYA [1] assumes that the fission fragments emerge with angular momenta that are perpendicular to the fission axis and they are therefore sampled from the corresponding 2D distribution. The resulting spin-spin opening-angle distribution [6] is then in accordance with the results sampled here, as shown in Fig. 3.

7 Concluding remarks

We presented a simple statistical model for the coupled angular momenta of the fission fragments and described two different but equivalent methods for sampling those, taking into account their correlations due to angular momentum conservation. These methods were applied to sampling the angular momenta of fission fragments in either three or two dimensions. With a focus on the distribution of the spin-spin opening angle ψ, it was illustrated how the magnitude of the moment of inertia for the relative motion influences $P(\psi)$ significantly.

Comparisons with recent model calculations of the opening-angle distribution showed that the result obtained with Antisymmetrized Molecular Dynamics [3] agrees well with the statistical form pertaining to 3D spins with realistic moments of inertia, as might be expected from the short mean free path of the wave packets. On the other hand, it is puzzling that results obtained with microscopic time-dependent functional theory [2] have a form similar to the 3D equlibrium distribution with a very small relative moment of inertia corresponding to a shape significantly more compact than touching spheres. With regard to both of these comparisons, it should be noted that the 3D samplings do not invoke the scission geometry and thus ignores the basic requirement that the relative angular momentum $\boldsymbol{S}_0 = \boldsymbol{R} \times \boldsymbol{P}$ be perpendicular to the fission axis $\boldsymbol{R}$. Therefore, agreement of a model with the 3D statistical samplings does not provide support for it.

It was shown experimentally long ago [8] that the fragment spins are preferentially perperdicular to the fission direction. This requirement reduces the samplings to 2D and it was shown that these slightly favor anti-parallel spins, $\psi \approx \pi$, with an amplitude of $\approx$10% when realistic scission configurations are used. Such 2D simulations reproduce the results of fission calculations with the FREYA code [6, 7] which does take account of the specific scission geometry and generates fragment spins that are perpendicular to the fission axis.

The present work brings out an important general feature of the coupled angular momenta appearing in fission: The relative motion, due to the large size of the associated moment of inertia in comparison with those of the individual fragments, $\mathcal{I}_0 \gg \mathcal{I}_\mathrm{f}$, effectively acts as a reservoir of angular momentum. Then the conservation of angular momentum has little effect on the fragment spins and they become nearly independent. Indeed, the angular momenta generated by FREYA are only slightly correlated with regard to both their directions and their magnitudes. The latter feature was recently observed experimentally [9].

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