Seminar at ECT* - workshop Nonequilibrium phenomena in superfluid systems

Determining Fission Fragment Spin Properties Using Projection Techniques

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TDHF



G. Scamps, C. Simenel, D. Lacroix, PRC 92, 011602(R) (2015).



TDHF

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Impact of pairing

Pairing is a lubricant for fission

Quasi-particle vacuum

$$|\Psi
angle = \prod_{lpha} (u_{lpha} + v_{lpha} a_{lpha}^{\dagger} a_{\overline{lpha}}^{\dagger})|-
angle$$

In the particular case of two particles and two states :

$$\begin{split} |\Psi\rangle &= (u_1 + v_1 a_1^{\dagger} a_1^{\dagger})(u_2 + v_2 a_2^{\dagger} a_2^{\dagger})|-\rangle \\ &= u_1 u_2|-\rangle + u_2 v_1 a_1^{\dagger} a_1^{\dagger}|-\rangle + u_1 v_2 a_2^{\dagger} a_2^{\dagger}|-\rangle + v_1 v_2 a_1^{\dagger} a_1^{\dagger} a_2^{\dagger} a_2^{\dagger}|-\rangle \end{split}$$



Projector on the good number of particles

$$\hat{P}(N) = \frac{1}{2\pi} \int_0^{2\pi} e^{i\varphi(\hat{N}-N)} d\varphi$$

$$\hat{P}(2)|BCS> = C'_{2}$$
 $(2>)$ $+ C'_{3}$ $(1>)$ $(1>)$

Projection technique (C. Simenel, PRL 105 (2010))

$$\hat{P}_B(N) = rac{1}{2\pi} \int_0^{2\pi} e^{i arphi(\hat{N}_B - N)} darphi$$
 $P_B(N) = \langle \Psi(t) | \ \hat{P}_B(N) | \Psi(t)
angle$



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Same projection technique for a BCS state

$$\begin{split} |\Psi(t)\rangle &= |\phi_1\rangle \otimes |\phi_2\rangle = \prod_{\alpha_1} (u_{\alpha_1} + v_{\alpha_1} a^{\dagger}_{\alpha_1} a^{\dagger}_{\dot{\alpha}_1}) \prod_{\alpha_2} (u_{\alpha_2} + v_{\alpha_2} a^{\dagger}_{\alpha_2} a^{\dagger}_{\dot{\alpha}_2})|-\rangle \\ \hat{P}_B(N) &= \frac{1}{2\pi} \int_0^{2\pi} e^{i\varphi(\hat{N}_B - N)} d\varphi \\ P_B(N) &= \langle \Psi(t) | \ \hat{P}_B(N) | \Psi(t) \rangle \end{split}$$



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 $^{46}Ca + ^{40}Ca$

Double projection technique for a BCS state

$$\mathcal{P}_B(\mathsf{N}) = rac{\langle \Psi(t) | \hat{\mathcal{P}}_B(\mathsf{N}) \hat{\mathcal{P}}(\mathsf{N}_0) | \Psi(t)
angle}{\langle \Psi(t) | \hat{\mathcal{P}}(\mathsf{N}_0) | \Psi(t)
angle}$$

 $^{46}Ca + {}^{40}Ca$



Double projection technique for a BCS state

 $P_B(N) = rac{\langle \Psi(t) | \hat{P}_B(N) \hat{P}(N_0) | \Psi(t)
angle}{\langle \Psi(t) | \hat{P}(N_0) | \Psi(t)
angle}$



Results

Effect of pairing on P_1 and P_2



Effect of initial pairing correlations :

- fragmentation of single particle occupation numbers
 - enhancement of P_{1n}
- non-zero two body correlations ($\kappa \neq 0$)
 - enhancement of P_{2n}

G. Scamps and D. Lacroix, PRC 87, (2013)

Spins of the fission fragments



J. N. Wilson, Nature, 590, 566 (2021)

- The average spin follows a sawtooth shape
- No correlations between the spins of the fragments

Spins are mostly perpendicular to the fission axis



FIG. 9. The points are the calculated populations of the various *m* substates of the 2¹ level in ¹⁴ Hig. These values were determined using the fitted experimental angular distribution of the 2ⁿ -0° γ ray. The solid line represents the predicted population of the m states as calculated from the statistical-model analysis of the deexcitation process using Eqs. (4) and (5) with an assumed value of B = 6 [Eq. (3)] for the initial angular momentum distribution.

J. B. Wilhelmy, E. Cheifetz, R. C. Jared, S. G. Thompson, H. R. Bowman, and J. O. Rasmussen Phys. Rev. C 5, 2041 (1972)

Literature

- Thermal excitations
- Quantum fluctuations
- Coulomb force
- Breaking of the neck



Illustration from B. John, J. Phys., 85, 2, (2015).





A. Bulgac, P. Magierski, Kenneth J. Roche, and I. Stetcu, PRL 116, 122504 (2016).

Projection method

Projection on the spin and K number (Projection of the spin on the fission axis)

$$\begin{split} \hat{P}_{MK}^{S} &= \frac{(2S+1)}{16\pi^2} \int \! d\Omega \mathcal{D}_{MK}^{S*}(\Omega) \, e^{i\alpha \hat{S}_z} e^{i\beta \hat{S}_y} e^{i\gamma \hat{S}_z}, \\ P(S_F, K_F) &= \langle \Psi | \hat{P}_{K_F K_F}^{S_F} | \Psi \rangle, \end{split}$$

Calculation of the overlap : G. F. Bertsch and L. M. Robledo, PRL 108, 042505 (2012)

$$\langle \Psi | \hat{R} | \Psi \rangle = \frac{(-1)^n}{\prod_{\alpha}^n v_{\alpha}^2} \mathrm{pf} \begin{bmatrix} V^T U & V^T R^T V^* \\ -V^{\dagger} R V & U^{\dagger} V^* \end{bmatrix}$$

Optimized Pfaffian calculation : M. Wimmer, ACM Trans. Math Softw. 38, 30 (2012).



G.scamps, I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, PRC 108 (6), L061602



G.scamps, I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, PRC 108 (6), L061602.



TDDFT (in 2022) vs Freya



A. Bulgac, I. Abdurrahman, K. Godbey, and I. Stetcu, Phys. Rev. Lett. 128, 022501(2022).

$$\varphi_{\mathit{HL}} = \arccos\left(\frac{\Lambda(\Lambda+1) - S_{\mathit{H}}(S_{\mathit{H}}+1) - S_{\mathit{L}}(S_{\mathit{L}}+1)}{2\sqrt{S_{\mathit{H}}(S_{\mathit{H}}+1)S_{\mathit{L}}(S_{\mathit{L}}+1)}}\right)$$

$$P(\Lambda, S_H, S_L) = \sum_{k_H k_L} \langle \Psi | \hat{P}_{0,0}^{\Lambda} \hat{P}_{K_H K_H}^{S_H} \hat{P}_{K_L K_L}^{S_L} | \Psi \rangle.$$

$$P(\Lambda, S_H, S_L) = \sum_{K_H K_L K'_H K'_L} (-1)^{K'_H - K_H + K'_L - K_L}$$

$$C^{\Lambda,0}_{S_{H},-\kappa_{H},S_{L},-\kappa_{L}}C^{\Lambda,0}_{S_{H},-\kappa_{H}',S_{L},-\kappa_{L}'}\langle\Psi|\hat{P}^{S_{H}}_{\kappa_{H}\kappa_{H}'}\hat{P}^{S_{L}}_{\kappa_{L}\kappa_{L}'}|\Psi\rangle$$



G.scamps, I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, PRC 108 (6), L061602.





Question

- How the quantal effects change this picture?
- How the geometry change the opening angle distribution assuming no correlation?



To get a 5 degrees angle between two spins require spins of 262 \hbar and 6565 \hbar for 1 degree



Non alignement of the spins

$$\Lambda = 10 \qquad S_{H} = 5 \qquad \qquad \begin{array}{c} S_{H} = 5 \\ S_{L} = 5 \end{array} \qquad \qquad \begin{array}{c} S_{H} = S_{H} + 1/2 \\ S_{L} = 5 \end{array} \qquad \qquad \begin{array}{c} S_{H} = S_{H} + 1/2 \\ S_{L} = S_{L} + 1/2 \\ \end{array} \qquad \qquad \begin{array}{c} S_{H} = S_{H} + 1/2 \\ S_{L} = S_{L} + 1/2 \end{array}$$

To get a 5 degrees angle between two spins require spins of 262 \hbar and 6565 \hbar for 1 degree





$$|\Psi\rangle = \sum_{S_H, \kappa_H, S_L, \kappa_L} c_{S_H, \kappa_H, S_L, \kappa_L} |S_H, \kappa_H, S_L, \kappa_L\rangle,$$

$$\begin{aligned} |c_{S_{H},\kappa_{H},S_{L},\kappa_{L}}|^{2} \propto & \delta_{\kappa_{H},0} \delta_{\kappa_{L},0} (2S_{H}+1) e^{\frac{-S_{H}(S_{H}+1)}{2\sigma_{H}^{2}}} \\ & \times (2S_{L}+1) e^{\frac{-S_{L}(S_{L}+1)}{2\sigma_{L}^{2}}}. \end{aligned}$$



G. Scamps, PRC 109, L011602 (2024).

Opening angle distribution - 3D uniform case



G. Scamps, PRC 109, L011602 (2024).

Opening angle distribution - 3D from TDDFT

 $\theta_{\rm F}$ [deg]





G. F. Bertsch, T. Kawano, and L. M. Robledo, PRC 99, 034603 (2019)

Problem of interpretation

- The spin cut-off distribution is already present in the ground state of even-even deformed nuclei if symmetry are not restored
- *Ĵ*² and *P*(*J*) are 2 and N-body operators
- Fragments do not rotate in dynamical approaches

Microscopic calculations - Limitations



Problem of interpretation

- The spin cut-off distribution is already present in the ground state of even-even deformed nuclei if symmetry are not restored
- \hat{J}^2 and $\hat{P}(J)$ are 2 and N-body operators
- Fragments do not rotate in dynamical approaches

Microscopic calculations - Limitations



G. F. Bertsch, T. Kawano, and L. M. Robledo, PRC 99, 034603 (2019)

Problem of interpretation

- The spin cut-off distribution is already present in the ground state of even-even deformed nuclei if symmetry are not restored
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- Fragments do not rotate in dynamical approaches

Uncertainty principle?

If the overlap is gaussian

$$\langle \Psi | \hat{R}(\theta) | \Psi \rangle = e^{-rac{ heta^2}{2\sigma_{ heta}^2}}$$

The projection gives,

$$P(J) = \frac{2J+1}{2\sigma_J^2} e^{-\frac{J(J+1)}{2\sigma_J^2}}$$

with $\sigma_J \sigma_{\theta} = 1$





S. Franke-Arnold, et al. New Journal of Physics 6, 103 (2004)

G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616(2023).

au = + 2

 $\frac{1}{\sqrt{4\pi}} \frac{\sqrt{15}}{2^{3/2}} \sin^2 \theta e^{+i2\theta}$

 $w = \pm 3$

Orientation pumping mechanism

Isotropic potential at scission



L. Bonneau, P. Quentin, and I. N. Mikhailov, PRC 75, 064313 (2007). For $\Delta \Theta = 1^{\circ}$, $\Delta L = 56\hbar$. For a nucleus, angular velocity $\omega = 10^{20}s^{-1}$



Premiers harmoniques sphérique

A1 = 0

 $\frac{1}{\sqrt{4\pi}}\sqrt{3}\cos\theta$

w = +1

 $\frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{2}}\sin\theta e^{i\phi}$

 $\frac{\sqrt{15}}{2}\cos\theta\sin\theta e$

w = -1

 $\frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{2}}\sin\theta e^{-i\phi}$

 $\frac{1}{\sqrt{4\pi}} \frac{\sqrt{15}}{302} \sin^2 \theta e^{-i2\theta} \frac{1}{\sqrt{4\pi}} \frac{\sqrt{15}}{2} \cos \theta \sin \theta e^{-i\theta} \frac{1}{\sqrt{4\pi}} \frac{\sqrt{5}}{2} \left(3 \cos^2 \theta - 1 \right)$

AV = -3

AI = -2

Main points

- Internal excitation (breaking of pairs)
- Spins are mainly perpendicular to the fission axis
- Uncorrelated magnitude and orientation of the spins

Outlook

- TD-GCM with rotated fragments
- Rotated fission system

Thank you

^{144}Ba + ^{96}Sr at 16 Fm, Θ_{ini} = 25 deg, Functional : Skyrme Sly4d

 $J_y(x, z)[h \ fm^{-3}]$

G. Scamps, PRC 106, 054614 (2022).

One body-evolution - One body-observable

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G. Scamps, PRC 106, 054614 (2022).

One body-evolution - One body-observable

Microscopic DFT calculations







Projection method

$$\hat{P}_{J}\left(|\Psi(J=0)
angle+|\Psi(J=1)
angle+...
ight)
onumber \ =|\Psi(J)
angle$$

$$\begin{split} |a_{J}^{F}|^{2} = & \frac{2J+1}{2} \int_{0}^{2\pi} \sin(\beta) \\ P_{J}(\cos(\beta)) \langle \Psi | e^{\frac{-iJ_{X}^{F}\beta}{\hbar}} | \Psi \rangle \end{split}$$

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G. Scamps, PRC 106, 054614 (2022).



Potential as a function of the light fragment angle

 $^{132}Sn + ^{108}Ru$



Two torques :

- attractive nucleus-nucleus torque
- repulsive Coulomb torque

Potential as a function of the light fragment angle



The azimuthal angle doesn't have an important role.

Frozen Hartree-Fock potential



Two torques :

- attractive nucleus-nucleus torque
- repulsive Coulomb torque



Hamiltonian

$$\hat{H}(D) = \frac{\hbar^2}{2I_H} \hat{L}_H^2 + \frac{\hbar^2}{2I_L} \hat{L}_L^2 + \frac{\hbar^2}{2I_h(D)} \hat{\Lambda}^2 + \hat{V}(\hat{\Theta}_H, \hat{\Theta}_L, \hat{\varphi}, D)$$
Solved in basis $|L_H, m, L_L, -m\rangle$

G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616(2023).

Similar to the orientation pumping mechanism model Mikhailov, I. N., and Quentin, P. Physics Letters B, 462(1-2), 7-13 (1999)



G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).





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G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).

Effect of quadrupole deformation >> effect of Z_1Z_2

TABLE II. Average spin $(L^2)^{\frac{1}{2}}$ in unit of \hbar for the three fission fragments at scission (D = 21 fm) and at large distances. The last two columns show the same quantity with an MOI divided by 2.

Nucleus	Scission	Final	Scission $(I_{\frac{1}{2}})$	Final $(I_{\frac{1}{2}})$
¹⁰⁸ Ru	9.28	12.31	7.24	10.38
¹⁴⁴ Ba	10.04	10.95	7.70	8.66
⁹⁶ Sr	7.74	9.30	6.03	7.62

also J. Randrup, PRC 108, 064606 (2023) : increase of 1 to 3 \hbar due to the Coulomb torque.



- ¹³²Sn is found in ground-state
- The collective Hamiltonian model with $\beta_2=0.42$ reproduces the experimental γ -spectrum



A. Francheteau, L. Gaudefroy, G. Scamps, O. Roig, V. Méot, A. Ebran, and G. Bélier, PRL 132, 142501 (2024).

Correlation between the angular momentum



¹⁴⁴Ba+⁹⁶Sr

- No or small correlation observed in the magnitude of the angular momentum.
- More angular momentum for the heavy fragment



Mechanism



- Pear-shaped deformation plays an important role at scission. G. Scamps C. Simenel, Nature 564, pages 382–385 (2018)
- Octupole deformation makes the angular potential stiffer which increase the zero-point motion → more angular momentum

G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).





G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).

Geometry

- Small azimuthal correlation
- Spins are perpendicular to the fission axis
- Complex pattern in the opening angle, different from previous model

Outlook : Case where total spin is not zero

 $^{208}Pb + ^{208}Pb$



⁵⁰Ca+¹⁷⁶Yb



G. Scamps, Microscopic Study of Spin Transfer in Near-Barrier Nuclear Reactions, Phys. Rev. C 110, 054605 (2024).

$^{208}Pb + ^{208}Pb$

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G. Scamps, Microscopic Study of Spin Transfer in Near-Barrier Nuclear Reactions, Phys. Rev. C 110, 054605 (2024).

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