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Collective mass parameters in Skyrme EDF

 Niigata Univ. Kenichi Yoshida Key ingredients for spontaneous fission in nuclear EDF

Collective Hamiltonian describing the fission dynamics

$$
\mathcal{H} = \frac{1}{2} \sum_{kl} M_{kl}(s) \dot{s}_k \dot{s}_l + V_{\text{coll}}(s)
$$

Dynamical variables $s = (s_1, s_2, \dots) = (\beta, \gamma, \beta_3, \dots)$

Collective potential $s = \frac{1}{\sqrt{2}}$ $V_{\text{coll}}(s)$

Inertia functions for the collective mode $\overline{M_{kl}}(s)$

Collective potential $\mathcal{L}(\mathcal{L})$ strength parameters fitted to reproduce the experimental to $\mathcal{L}(\mathcal{L})$ \mathbf{D} Nect, ive dotent $t = 0$ developed multipliers cases, a continuous path may even cross a higher saddle point. Although the spurious saddle points may not be excluded completely, most of them can be avoided if (i) the obtained

$I_n = \frac{1}{2}$ dimensional collective space. To separate fission pathways, we computed the deformation surfaces in the deformation spaces in the deformation spaces in the deformation sp self-consistent values of multipole moments, the nonuniform \checkmark potential energy surface in multi-dimensional constrained EDF method 0.9 (around the fission isomer), 1.3 (around the second saddle position direction the ground state and the fission is a state and the fission is a state and the fission is a state and the fission of \sim reflection symmetric as what is shown in the 1D PEC and r_{max} are examined by \mathbf{r}_{max} have carefully checked the full 3D PES and found that the fission path enters and exits the triaxial configuration rather

point, defined by the set of constrained multipole moments, $f + \Omega T$ of the Gogny

 $\mathbf{I} \cdot \mathbf{n} = \mathbf{I} \cdot \mathbf{n}$ lower-dimensional constraint calculation is a necessary but

relativistic Gogny Skyrme finds that the stiffness of the fission isomer is much larger $t = 20002 + 20002$

0.8 $\beta_{20} = 0.3 + \beta_{20} = 0.6$ \sim the smallest field field finallel that \sim $\text{O.O}\left(\text{O}\left(\text{O}\left(\text{O}\left(\text{O}\left(\text{O}\left(\text{O}\right) \right) \right) \right) \right) \text{N} \right)$ \mathbb{Z} in Eq. (2) can be seen as a line integral of the function \mathbb{Z} -0.4 -0.4 surface delimited by this line and the x axis provides the value of the action S. In panel (h) we display dS(Q2)/dQ² $\beta_{20} = 0.9 + 1.3 + 1.3 + 1.3$ t the t final path t final path t fission t final path t $\mathcal{A} \subset \mathbb{R}$ that are actions $\mathcal{A} \subset \mathbb{R}$ for $\mathcal{A} \subset \mathbb{R}$, then both approximate are actions of $\mathcal{A} \subset \mathbb{R}$ β_{30} very computation of the actual values of S are 26.69 (AS-RS) and 26.69 (AS-RS) and 26.69 (AS-RS) and 26.69 (AS- 2.64 (NAS-RS), which is the AS-NRS case we obtain a much similar weight of \sim larger value, namely 41.66. In the nucleus 278Ds, the fission p_{10} and the p_{20} paths alone with the \sim approximately with the process would provide much shorter than the shorter lifetimes that the shorter lifetime AS-RS one. However, in panel (h) one finds that the three are rather similar similar. Actually, the precise \mathbb{R}^n $\|A\|$, and $\|A\|$ and $\|A\|$, and $\|A\|$, $\|A\|$ and $\|A\|$ show this show that $\|A\|$ to be the case. Let us a contribution of the prediction of the final prediction of the prediction of the final paths is more or less in accordance with the one of panel (h) and the actual numbers 23.34 (AS-RS), 18.32 (AS-NRS), and $r_{\rm c2}$ for any $r_{\rm g2}$ and $r_{\rm g2}$ a Ω and ρ $240D_1$ approximation, though as we we will see later one can find

\Box \Box the QXVI.IIIA different energy surfaces locally valid around each fission

configuration associated with two touching, nearly spherical, nearly spherical, nearly spherical, nearly spherical, $\mathcal{L}(\mathbf{D})$ Z hao, Z hou, $\mathrm{PRC85(2012)}$ 011301(R) $\sum_{i=1}^n a_i$ and $\sum_{i=1}^n a_i$ is $\sum_{i=1}^n a_i$ we expect the finding $\sum_{i=1}^n a_i$ state), 0.6 (around the first saddle point), 0.9 (around the fission Lu, Zhao, Zhou, PRC85(2012)011301(R) $\mathcal{L}(\mathbf{n})$

Staszczak, Baran, Dobaczewski, $\sum_{i=1}^{n}$. The fission pathways are marked: symmetric compact fragments. Nazarewicz, PRC85(2012)024314

All those studies were symmetry-restricted (i.e., they did not consider simultaneous inclusion of elongation, triaxiality, and reflection-asymmetry). that one could switch from one path to the other without further problem. However, if we look at a higher dimensional plot one can see the case. This is no thing drawn in Fig. 8 potential energy contour lines versus the quad r_1 toward a class-3 PES (talk by Dubray) and the AS-NRS paths of Fig. 7 for the respective nucleus. The \Box an andr τ and \Box of alter \gtrsim N bort tanger been set at the energy minimum. present a well-prolate-deformed minimum around 15 b. In √continuous potential energy surface

Microscopic collective-mass parameter For instance, in Ref. [11], time-odd fields have been included lin the Haroscopic collective-mas time-odd fields have also been incorporated in the HFB study and the collective mass tensor te $\frac{1}{2}$

\sim \cap \cap \cap \cap \cap \sim \sim \sim \sim \sim \bullet GCM-GOA mas ¤ ⊺
∃ ∕±±∪∪±
NASS • GCM-GOA mass

III. APPROXIMATIONS TO ATTEND TO ATTEND TO ATTEND THE REPORT OF ATTENDING Then, in terms of the corresponding matrices \mathcal{F}_n and \mathcal{F}_n , then \mathcal{F}_n exact calculation (talk by Robledo)

• ATDHFB mass \bullet ATDHFB mass

$$
\mathcal{M}_{ij} = \frac{i}{2\dot{q}_i\dot{q}_j} \text{Tr}(F^{i*}Z^j - F^i Z^{j*}).\tag{34}
$$

time-odd fields neglected Baran, Sheikh, Dobaczewski, Nazarewicz, basis from time-odd fields neglected Staszczak, PRC85(2012)024314 $\mathbf{D} = \begin{bmatrix} 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 &$ Staszczak, PRC85(2012)024314 $T_{\rm eff}$ for the expression (34) for the mass tensor contains the mass tensor contains the mass tensor contains the matrix Δt 1 and Bara
1 and Stas $\sum_{i=1}^n$

αβ = (Eβ)Zi Cranking approximation

$$
\mathcal{M}_{ij}^C = \frac{1}{2\dot{q}_i\dot{q}_j} \sum_{\alpha\beta} \frac{\left(F_{\alpha\beta}^{i*} F_{\alpha\beta}^j + F_{\alpha\beta}^i F_{\alpha\beta}^{j*} \right)}{E_{\alpha} + E_{\beta}} \qquad \qquad \sum_{\alpha=0}^{5} \frac{0.04}{0.03} \bigg|^{(a)}
$$

 Ω is shown being that Eq. (35) is diagonal in the Ω

The perturbative cranking expression for the mass tensor for the mass tensor for the mass tensor for the mass

 $\mathcal{L}_\mathbf{R}$, in the absence of the absence of the absence of the term involving $\mathcal{L}_\mathbf{R}$

b Perturbative cranking in put to the ATDHFB-C mass tensor (36) is the matrix F. $T_{\rm eff}$, and the perturbative cranking expression for the mass tensor tensor tensor for the mass tensor tensor $T_{\rm eff}$ rende and **Leu**d ${\rm Perturbative\hspace{0.1cm}cranking} \hspace{2.5cm} \mathfrak{L} \hspace{2.5cm} 0.02 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

(^ρ⁰ ^κ⁰

$$
\mathcal{M}^{C^{p}} = \frac{1}{4} [M^{(1)}]^{-1} M^{(3)} [M^{(1)}]^{-1}
$$

$$
M_{ij}^{(K)} = \sum_{\alpha\beta} \frac{\langle 0 | \hat{Q}_{i} | \alpha\beta \rangle \langle \alpha\beta | \hat{Q}_{j}^{\dagger} | 0 \rangle}{(E_{\alpha} + E_{\beta})^{K}}
$$

)

,

Local QRPA method \tilde{a}

Hinohara, Sato, Nakatsukasa, Matsuo, Matsuyanagi, PRC82(2010)064313

CHFB eq. $\delta \langle \phi(s)|\hat{H}_{\text{CHFB}}|\phi(s)\rangle = 0$ 2 i kl $\hat{H}_{\text{CHFB}} = \hat{H}_{\text{HFB}} - \sum$ i $\mu_i \hat{s}_i$

 $|\phi(s)\rangle$ ∂s^k $s) \rangle$ kl
kl $V_{\text{coll}}(s) = \langle \phi(s) | \hat{H}_{\text{HFB}} | \phi(s) \rangle$

Local harmonic approximation at each state $|\phi(s)\rangle$

$$
\delta \langle \phi(s) | [\hat{H}_{\text{CHFB}}, \hat{Q}_{\mu}(s)] - \frac{1}{i} \hat{P}_{\mu}(s) | \phi(s) \rangle = 0
$$

$$
\delta \langle \phi(s) | [\hat{H}_{\text{CHFB}}, \frac{1}{i} \hat{P}_{\mu}(s)] - C_{\mu}(s) \hat{Q}_{\mu}(s) | \phi(s) \rangle = 0
$$

✦collective mode generated self-consistently \blacklozenge time-odd effects taken into account ˆ CHFB|φ(s)"

Collective kinetic energy

$$
\mathcal{T} = \frac{1}{2} \sum_i (\dot{q}_i)^2
$$

=
$$
\frac{1}{2} \sum_i \sum_{kl} \frac{\partial q_i}{\partial s_k} \frac{\partial q_i}{\partial s_l} \dot{s}_k \dot{s}_l \equiv \frac{1}{2} \sum_{kl} M_{kl}(s) \dot{s}_k \dot{s}_l
$$

Note that the infinitesimal displacement of the collective coordinates brings about a corresponding change; α cement of th $\overline{\text{S}}$ $\frac{1}{2}$ ective coordinates brings about

$$
ds_k = \sum_i \frac{\partial s_k}{\partial q_i} dq_i
$$

derivative w.r.t. the collective coordinate q_i q_i

$$
\begin{aligned} \frac{\partial s_k}{\partial q_i} &= \frac{\partial}{\partial q_i} \langle \phi(s) | \hat{s}_k | \phi(s) \rangle \\ &= \langle \phi(s) | \left[\hat{s}_k, \frac{1}{i} \hat{P}_i(s) \right] | \phi(s) \rangle \\ &\quad \text{not in need of} \end{aligned}
$$

not in need of numerical derivative ^k|φ(s)"

Numerical implementation with use of Skyrme EDF Skyrme + pairing EDF: $\ E[\varrho(\bm{r}), \tilde{\varrho}(\bm{r})]$ KY, Hinohara, PRC83(2011)061302(R)

CHFB eq. in cylindrical coordinates assuming the axial, reflection symmetries

$$
\left(\begin{matrix} h(\bm{r}\sigma)-\lambda & \tilde{h}(\bm{r}\sigma)\\ \tilde{h}(\bm{r}\sigma) & -h(\bm{r}\sigma)+\lambda \end{matrix}\right) \left(\begin{matrix} \varphi_{1,\alpha}(\bm{r}\sigma)\\ \varphi_{2,\alpha}(\bm{r}\sigma) \end{matrix}\right)=E_\alpha \left(\begin{matrix} \varphi_{1,\alpha}(\bm{r}\sigma)\\ \varphi_{2,\alpha}(\bm{r}\sigma) \end{matrix}\right)\qquad \bm{r}=(\rho,z,\phi)
$$

Mean field (ph) and pair field (pp): $\,\beta$ constraint

$$
h=\frac{\delta E}{\delta \varrho}-\mu q_{20},\qquad \quad \tilde{h}=\frac{\delta E}{\delta \tilde{\varrho}}
$$

LQRPA eq. in the matrix form (P-Q representation)

$$
(A - B)Q_{\mu} = \frac{1}{i}P_{\mu}
$$

$$
(A + B)\frac{1}{i}P_{\mu} = \omega_{\mu}^{2}Q_{\mu}
$$

$$
(A+B)(A-B)Q_{\mu} = \omega_{\mu}^2 Q_{\mu}
$$

applicable to the situation where the eigen-frequencies of the local normal modes are imaginary

Quadrupole collective mass $\ M_{\beta\beta}(\beta)$ in the LQRPA $\overline{}$)
1 \mathbf{r} $\overline{ }$ $\overline{\mathbf{R}}$ ω u Bαα!(β) e d

•choose "the most collective mode" out of numerous eigenmodes αα!

practically, the mode possessing the smallest quadrupole mass in the low-frequency region of $\;\omega_i^2 < 15\;\, {\rm MeV}^2$

•calculate the quadrupole collective mass

$$
M_{Q_{20}Q_{20}}(\beta) = \left(\frac{dq_i}{dQ_{20}}\right)^2
$$

\n
$$
= \left| \langle \phi(\beta) | [\hat{Q}_{20}, \frac{1}{i} \hat{P}_i(\beta) | \phi(\beta) \rangle \right|^{-2}
$$

\n
$$
= \left[\frac{2}{i} \sum_{\alpha \alpha'} q_{20, \alpha \alpha'} P_{i, \alpha \alpha'}(\beta) \right]^{-2}
$$

\n
$$
= \left[\sum_{\alpha \alpha'} B_{\alpha \alpha'}(\beta) \right]^{-2}
$$

\n
$$
= \left[\sum_{\alpha \alpha'} B_{\alpha \alpha'}(\beta) \right]^{-2}
$$

 $B_{\alpha\alpha'}(\beta)$ Microscopic structure of the collective mass

CHFB calculation: MPI parallelization

use of N processors

QRPA calculation on parallel computer: MPI and BLACS

QRPA: use of N processors

 $A_{\alpha\beta\gamma\delta}$ $B_{\alpha\beta\gamma\delta}$ matrix elements of the QRPA eq.:

ScaLAPACK

2D-block cyclic distribution for load balancing

function: indxl2g for distribution subroutine: pdsyev for diagonalization

Ex. dim. : 50,000 for K=0 in 240Pu

w/ 512 cores 1024 cores 2048 cores

matrix element: 14,000 secs 7,000 secs 3,600 secs diagonalization: 1,400 secs 740 secs 680 secs inversion : 21 secs 15 secs 13 secs

Numerical results for 240Pu: Potential energy

SkM* +

pairing EDF

Yamagami, Shimizu, Nakatsukasa, PRC80(2009)064301

adjusted to pairing properties of welldeformed nuclei

Quadrupole mass parameter in 240Pu

strong dependence on the shell structure/ configuration

curvature of the collective potential $C_i(\beta) = \omega_i^2(\beta)$

Microscopic structure of collective mass in 240Pu

Enhanced collective mass

LQRPA and ATDHFB-Cranking masses in ²⁵⁶Fm Date in step of 1 and 3 b. The steps of 1 and 3 b. The design steps of 1 and 3 b. The design steps of 1 and 3 b. The design step of 1 and in HFB/HF+BCS were taken to compute the mass tensor, i.e., nea and airpe

SkM* + mixed-type pairing and the consistent solutions of Λ TDHFB: several neighboring deformation points. We have evaluated the

Baran, Sheikh, Dobaczewski, Nazarewicz, Staszczak, PRC85(2012)024314

using HFODD

Summary

Collective mass parameters for the quadrupole vib. calculated by use of the LQPRA method w/Skyrme EDF V LUUUU UU
Stariata mass j

Time-odd components are included

strongly dependent on the structure of the vacua

more than twice at most as large as the perturbative-cranking mass $0\hbar\omega$ 2qp excitation sensitive to the shell structure

Perspective

Deeper understanding of the mass parameter microscopically in terms of the quasiparticle excitation

Benchmark is needed

among the LQRPA, ATDHFB(-Cranking), GCM-GOA masses Quadrupole mass parameters on the symmetric path way

Application to spontaneous fission dynamics LQRPA on top of the triaxial and octupole deformed states

3D-QRPA code is needed

HFODD + parallelized m-FAM may be a practical way for it(?) m-FAM: Avogadro, Nakatsukasa, PRC87(2013)014331