Approximate symmetry restoration correction at the SR level with the Lipkin method

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The Lipkin method

As demonstrated by Lipkin in 1960, the minimized energy, obtained by the full variation after the particle-number projection (VAPNP), can also be obtained through an auxiliary Routhian,

$$\hat{H}' = \hat{H} - \hat{K}\{\hat{N} - N_0\}\,,$$

where Lipkin operator $\hat{K}$, which is a function of the shifted particle-number operator $\hat{N} - N_0$, is chosen so as to "flatten" the N-dependence of average Routhians calculated for the particle-number projected states. Had these projected Routhians been exactly N-independent (perfectly flat), the exact projected energy E_{N_0} could have been obtained by minimizing the average value of the Routhian for the unprojected state $|\Phi\rangle$, that is,

$$E_{N_0} = \langle\Phi|\hat{H} - \hat{K}\{\hat{N} - N_0\}|\Phi\rangle\,.$$

Otherwise, the Lipkin method gives an approximate VAPNP energy, and its accuracy depends on the quality of the choice made for the Lipkin operator $\hat{K}$.

H. J. Lipkin, Ann. Phys. 9, 272 (1960)

The Lipkin method

As suggested by Lipkin, the simplest and manageable ansatz for the Lipkin operator $\hat{K}$ has the form of a power expansion,

$$\hat{K}\{\hat{N} - N_0\} = \sum_{m=1}^{M} k_m (\hat{N} - N_0)^m \,,$$

where $k_1 \equiv \lambda$ is the Fermi energy. Up to now, the LN method was frequently used to estimate values of $k_2 \equiv \lambda_2$). However, this method relies on calculating the average values of $\langle \Phi | \hat{H} \hat{N}^m | \Phi \rangle$ and $\langle \Phi | \hat{N}^m | \Phi \rangle$, and, thus, at higher orders ($m > 2$) evaluation of these terms becomes cumbersome and impractical.

The original Lipkin method relies on deriving expressions for k_m that "flatten" the ϕ-dependence of the reduced Routhian kernel $h'(\phi)$, that is,

$$h'(\phi) = h(\phi) - \sum_{m=1}^{M} k_m n_m(\phi) \,,$$

where $H(\phi) = \langle \Phi | \hat{H} | \exp\left(i\phi(\hat{N} - N_0)\right) | \Phi \rangle$ and

$$h'(\phi) = \frac{H'(\phi)}{I(\phi)} \,, \quad h(\phi) = \frac{H(\phi)}{I(\phi)} \,, \quad n_m(\phi) = \frac{N_m(\phi)}{I(\phi)} \,.$$

H. J. Lipkin, Ann. Phys. 9, 272 (1960)

The Lipkin method

Lipkin parameters k_m for $m = 1, \ldots, M$ can be determined by requiring that equations are fulfilled at gauge angle $\phi = \phi_0 = 0$ and also at all M other nonzero values of the gauge angle ϕ_i. This gives

$$C + \sum_m k_m n_m(\phi_i) = h(\phi_i)\,,$$

where C is the flattened Routhian. Then, at sixth order, Lipkin parameters k_m can be easily obtained by inverting the matrix built of coefficients $n_m(\phi_i)$ as

$$\begin{pmatrix} C \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ k_5 \\ k_6 \end{pmatrix} = \begin{pmatrix} 1 & n_1(0) & \cdots & n_6(0) \\ 1 & n_1(\phi_1) & \cdots & n_6(\phi_1) \\ 1 & n_1(\phi_2) & \cdots & n_6(\phi_2) \\ 1 & n_1(\phi_3) & \cdots & n_6(\phi_3) \\ 1 & n_1(\phi_4) & \cdots & n_6(\phi_4) \\ 1 & n_1(\phi_5) & \cdots & n_6(\phi_5) \\ 1 & n_1(\phi_6) & \cdots & n_6(\phi_6) \end{pmatrix}^{-1} \begin{pmatrix} h(0) \\ h(\phi_1) \\ h(\phi_2) \\ h(\phi_3) \\ h(\phi_4) \\ h(\phi_5) \\ h(\phi_6) \end{pmatrix} .$$

At lower orders, or when neglecting odd orders, a smaller number of the gauge angle points can be used.

X.B. Wang *et al.*, Phys. Rev. C 90, 014312 (2014)

Convergence wrt maximum gauge angle

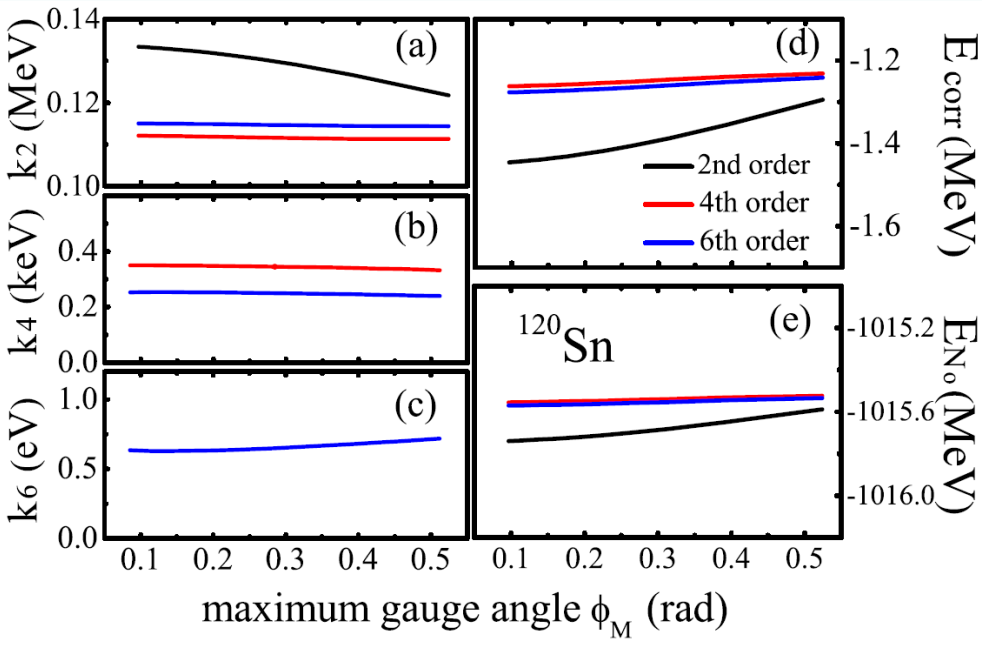

FIG. 1. (Color online) Lipkin parameters (a) k_2, (b) k_4, and (c) k_6, (d) Lipkin correction energy $E_{\rm corr}$, (16), and (e) Lipkin VAPNP energy E_{N_0}, (7), determined in ^{120}Sn at the second, fourth, and sixth orders, as functions of the maximum gauge angle ϕ_M. Note that Lipkin parameters k_2, k_4, and k_6 are shown in units of MeV, keV, and eV, respectively, which illustrates the rapid convergence of the Lipkin expansion.

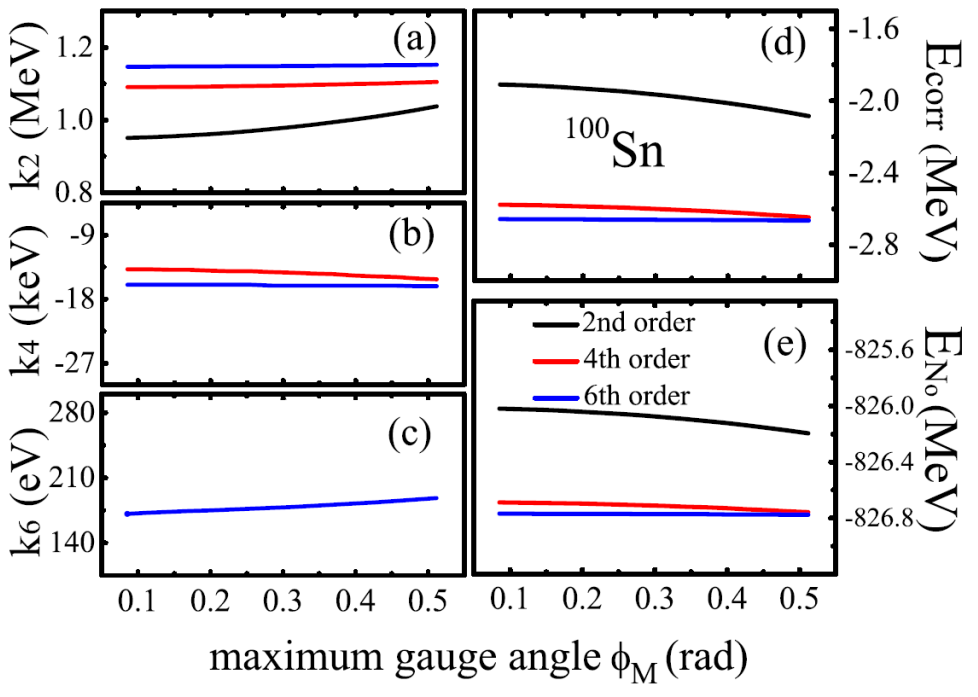

FIG. 2. (Color online) Same as Fig. 1, but for ^{100}Sn.

X.B. Wang *et al.*, Phys. Rev. C 90, 014312 (2014)

The energy kernels

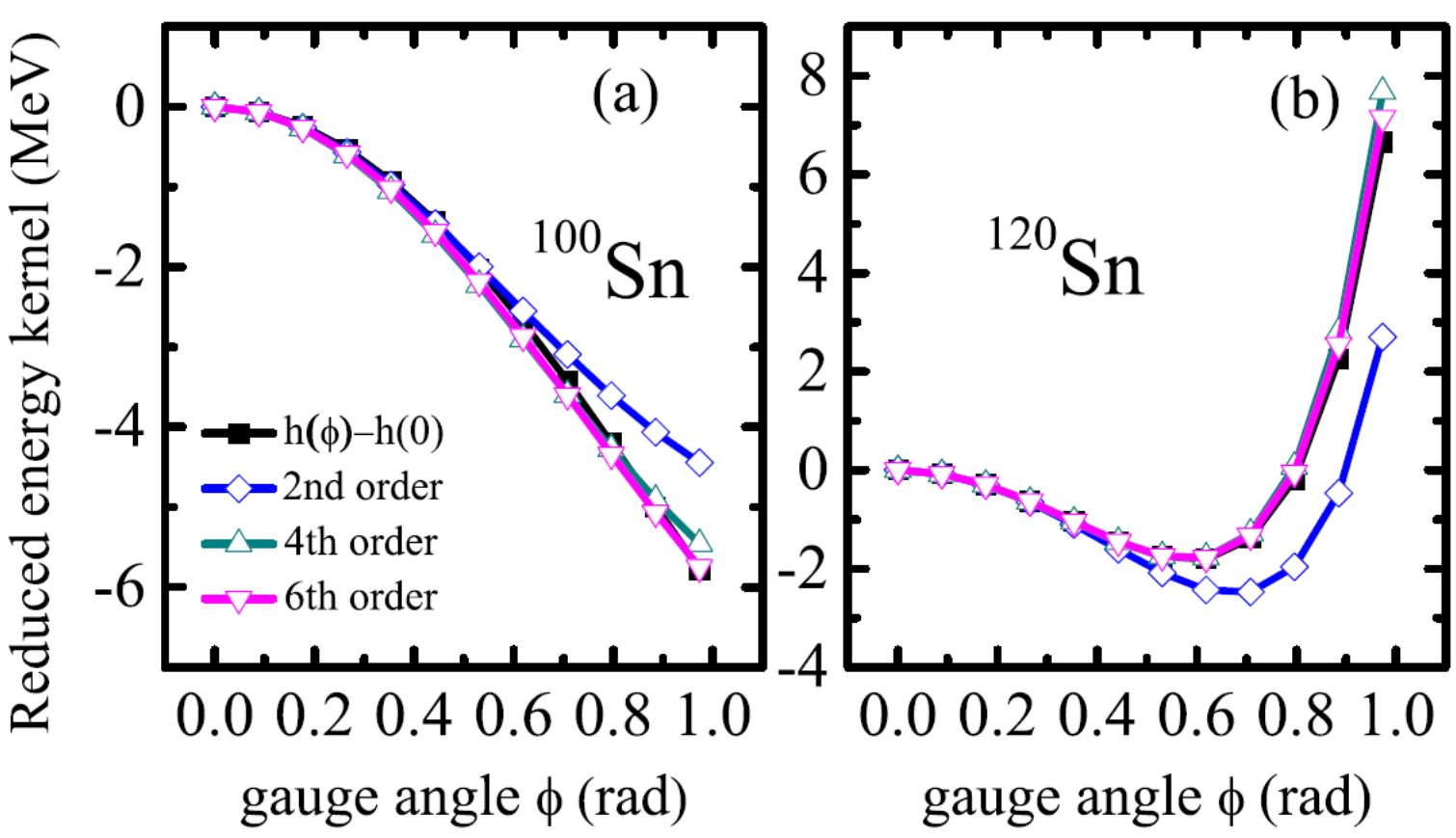

FIG. 3. (Color online) Reduced energy kernel $h(\phi) - h(0)$ (filled squares) and reduced kernels of the Lipkin operator $\sum_{m=1}^{M} k_m(n_m(\phi) - n_m(0))$ at orders $M = 2$, 4, and 6 (open symbols), as functions of the gauge angle up to $\phi = 1$, calculated in ^{100}Sn and ^{120}Sn.

X.B. Wang *et al.*, Phys. Rev. C 90, 014312 (2014)

The energy kernels

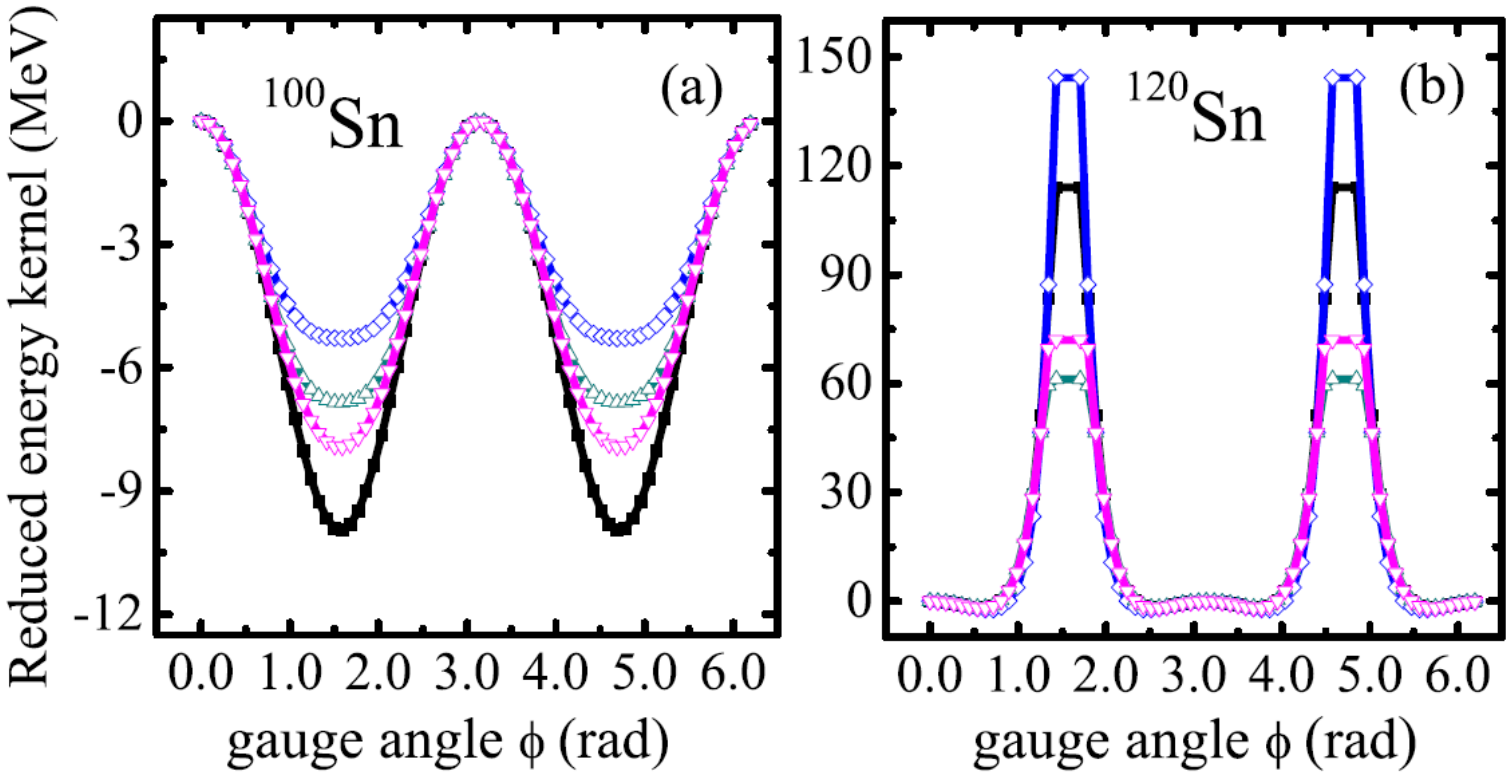

FIG. 4. (Color online) Same as Fig. 3, but for gauge angles up to $\phi = 2\pi$.

The Lipkin method regularizes the $3s_{1/2}$ pole at $\phi=\pi/2$

X.B. Wang *et al.*, Phys. Rev. C 90, 014312 (2014)

Projected energies in tin isotopes

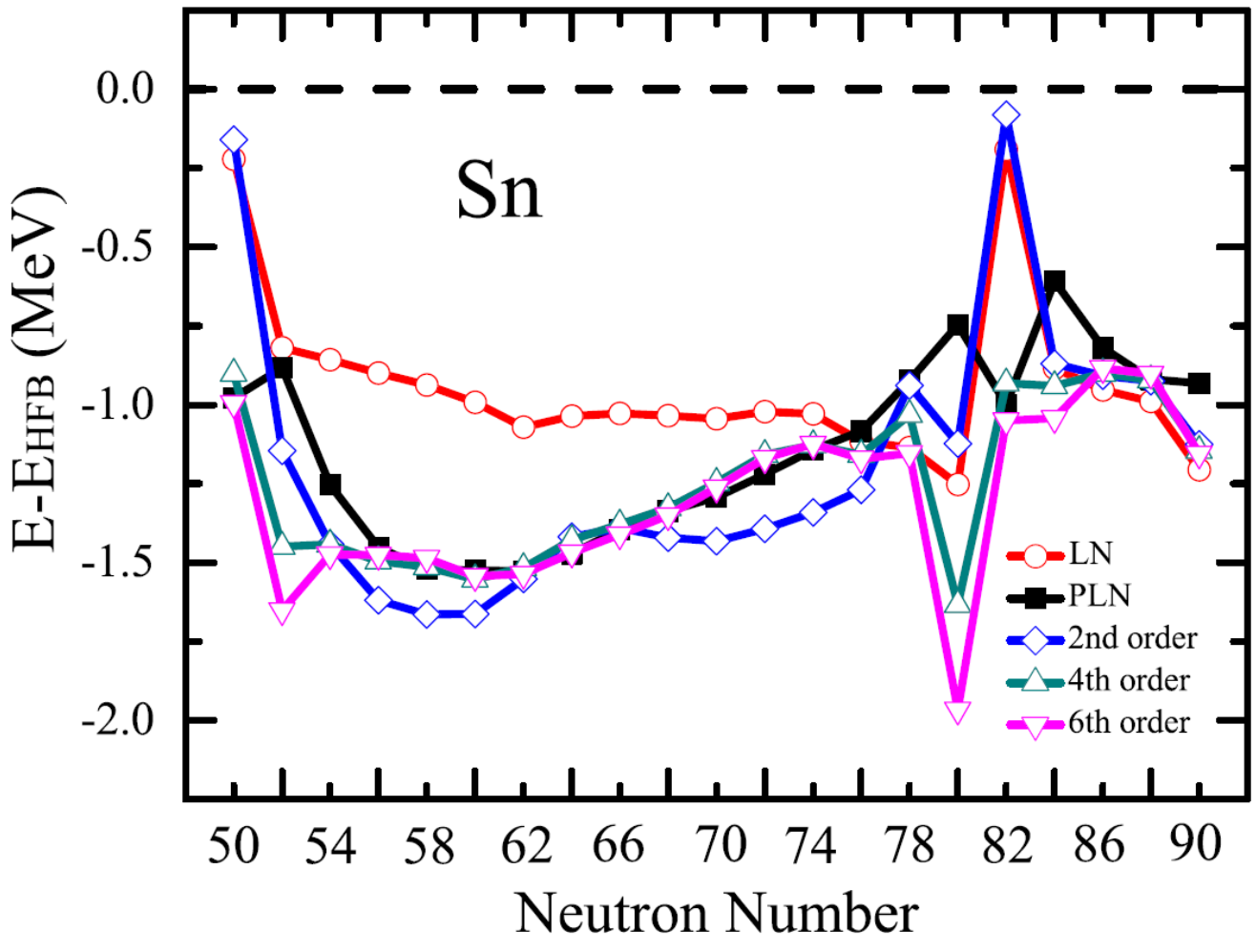

FIG. 5. (Color online) LN, PLN, and Lipkin VAPNP energies of tin isotopes relative to those obtained within the standard HFB method.

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Two-level pairing model

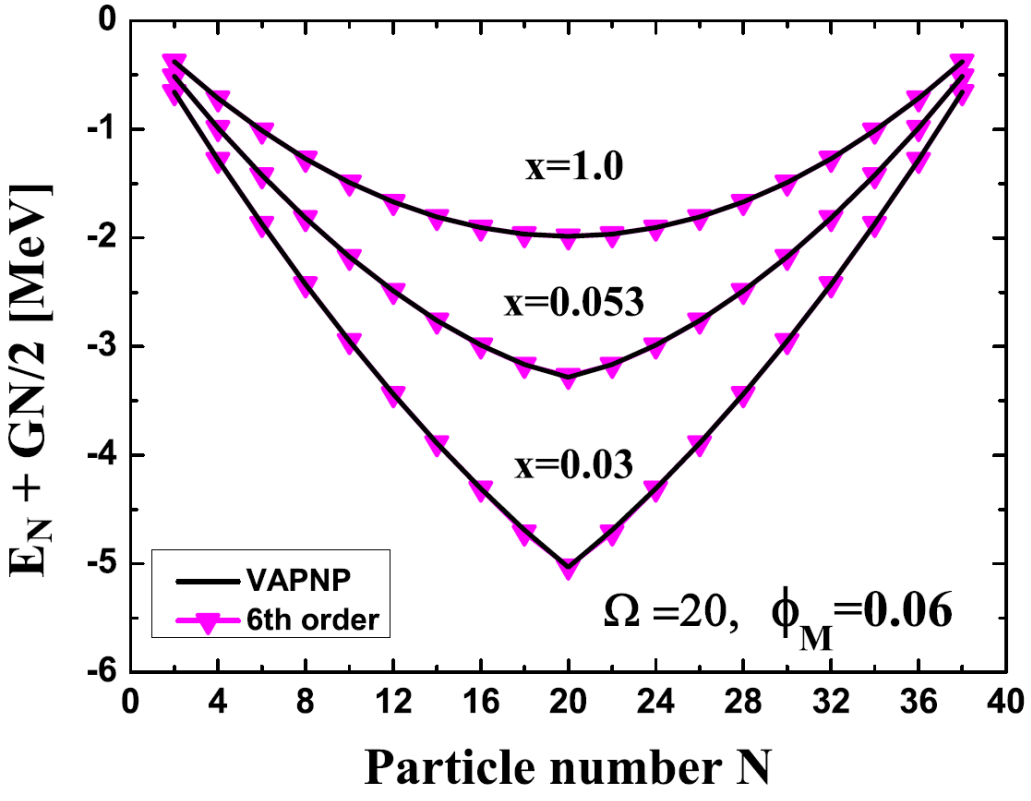

FIG. 9. (Color online) Ground-state energies in the two-level pairing model calculated within the sixth-order Lipkin and exact VAPNP methods. To render the curves symmetric with respect to the closed shell at $N = 20$, the appropriate linear term was added. Normalization of $50G + \epsilon = 1$ MeV was used.

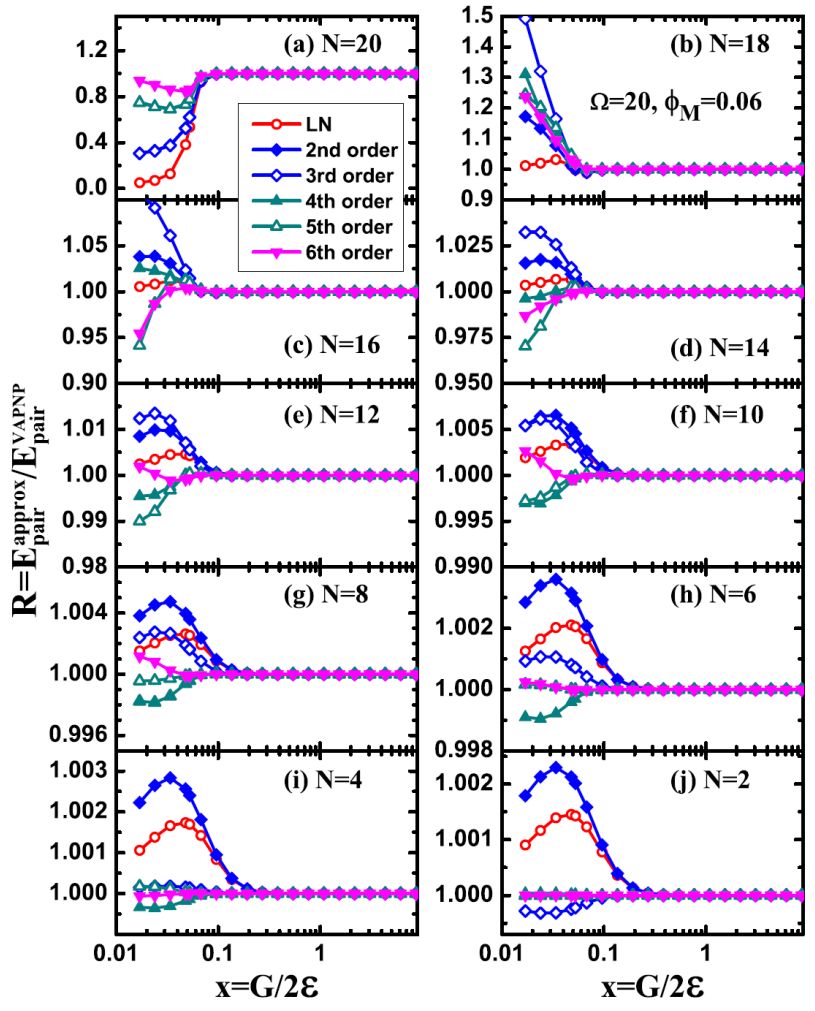

FIG. 10. (Color online) Ratios of approximate pairing energies, calculated within the approximate LN (open circles) and Lipkin VAPNP methods, relative to those of the exact VAPNP method. The figure shows results obtained for $\phi_M = 0.06$ as a function of the pairing-strength parameter $x = G/2\epsilon$. Note that (a)–(j) are drawn on very different scales, indicating the discrepancies of up to 100% for $N = 20$ and only 0.2% for $N = 2$.

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Translational and rotational symmetries

For the translational-symmetry restoration, $K\left[\hat{O}\right]$, $\hat{Q}$, and q are chosen as:

$$K[\hat{O}] = \sum_{i=x,y,z} k_i \hat{P}_i^2, \quad \hat{Q} = \hat{P}_{i=x,y,z}, \quad q = \delta x, \delta y, \delta z,$$

where $\hat{P}_i$ are components of the total momentum operator in three Cartesian directions. In this way, for $i = x, y, z$, operator $e^{iq\hat{Q}}$ shifts the nucleus by the distance of $\delta x, \delta y, \delta z$ in the direction of the x, y, z axis, respectively.

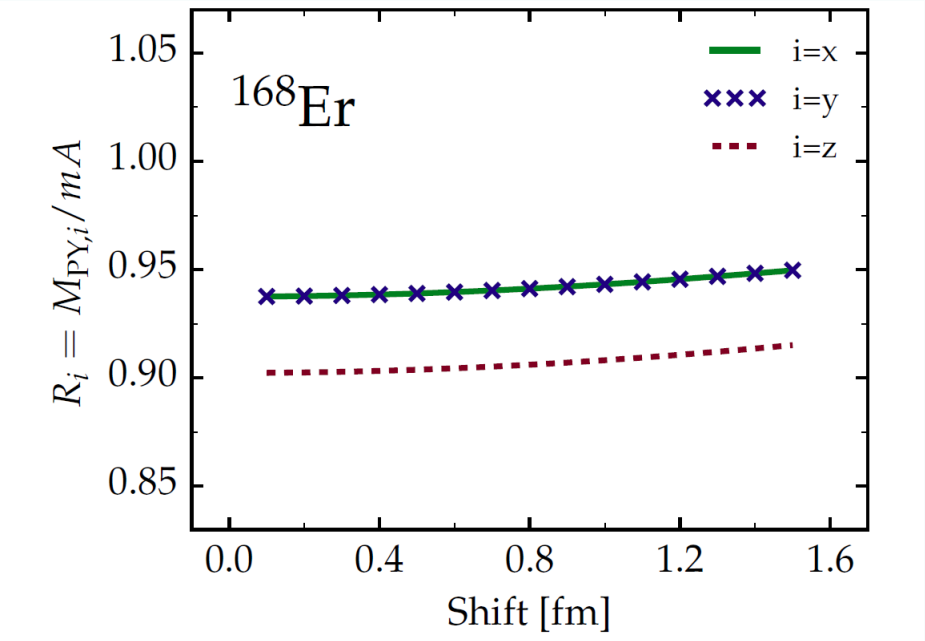
For the rotational-symmetry restoration, we concentrate on axially deformed even-even nuclei. Therefore, $K\left[\hat{O}\right]$, $\hat{Q}$, and q are now chosen as:

$$K[\hat{O}] = k\left(\hat{J}_x^2 + \hat{J}_y^2\right), \quad \hat{Q} = \hat{J}_y, \quad q = \beta,$$

where the axial-symmetry axis is aligned with the Cartesian z direction, $\hat{J}_x$ and $\hat{J}_y$ are the x and y components of the total angular momentum, respectively, and β is the Euler rotation angle about the y-axis.

Y. Gao *et al.*, arXiv:1511.02814v2

Peierls-Yoccoz masses



We represent the calculated values of Lipkin parameters k_i through the ratios of the corresponding Peierls-Yoccoz and exact masses, that is,

$$R_i = \frac{M_{\mathrm{PY},i}}{mA} = \frac{1}{2k_i mA} \quad \text{for} \quad i = x, y, z.$$

Needless to say that in deformed nuclei, the momentum contents in the three Cartesian directions of the intrinsic system can be different, and thus the three Peierls-Yoccoz masses $M_{\mathrm{PY},i}$ can be different too.

Y. Gao *et al.*, arXiv:1511.02814v2

Translational-symmetry restoration

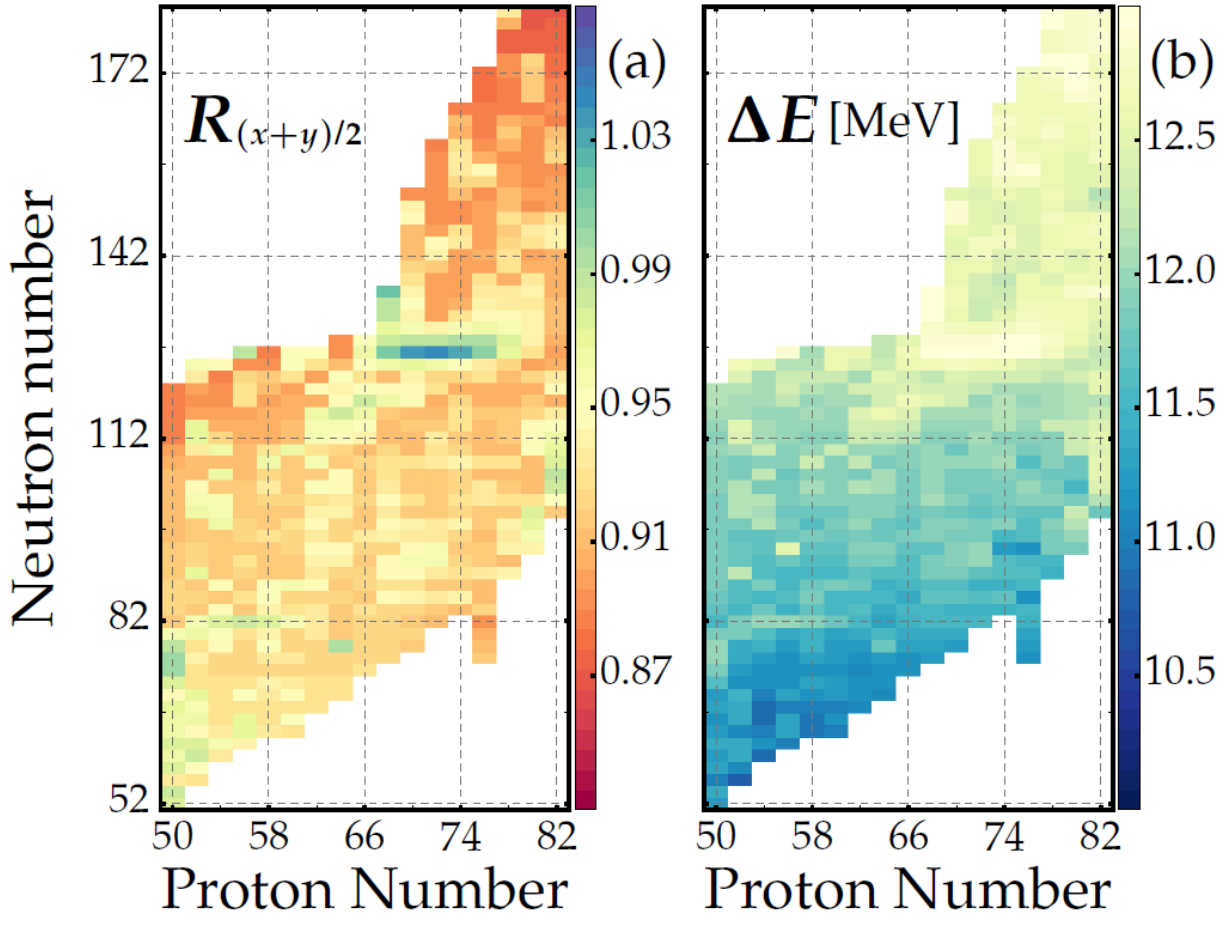


FIG. 2: (a) Average ratios of the Peierls-Yoccoz and exact masses in the x and y directions (18). (b) Differences ΔE between the Lipkin VAP energies and those obtained within the standard HFB calculations.

Y. Gao *et al.*, arXiv:1511.02814v2

Translational-symmetry restoration

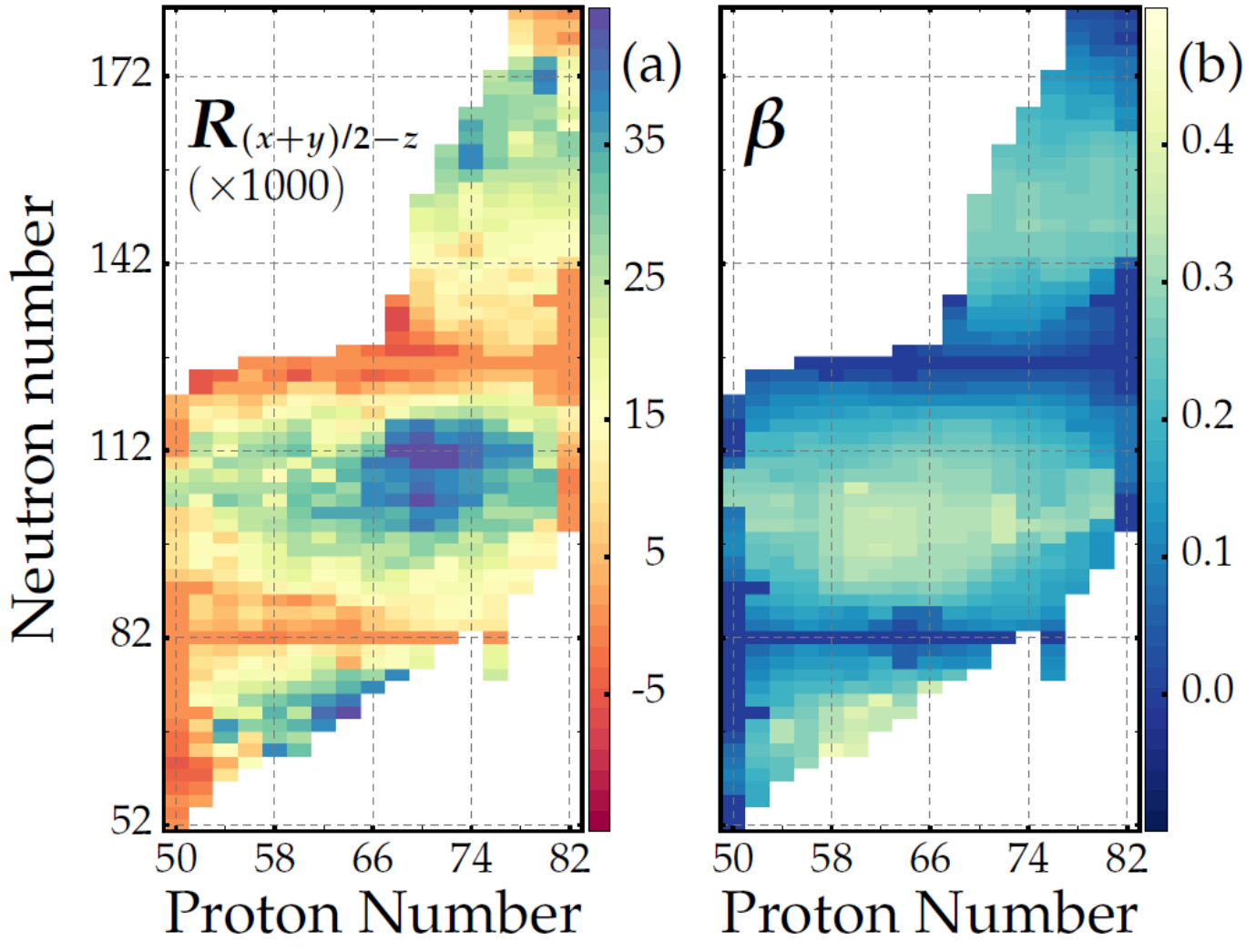


FIG. 3: (a) $R_{(x+y)/2} - R_z$: The difference between $R_{(x+y)/2}$ and the mass ratio in the z-direction. (b) Beta deformations.

Y. Gao *et al.*, arXiv:1511.02814v2

Translational-symmetry restoration

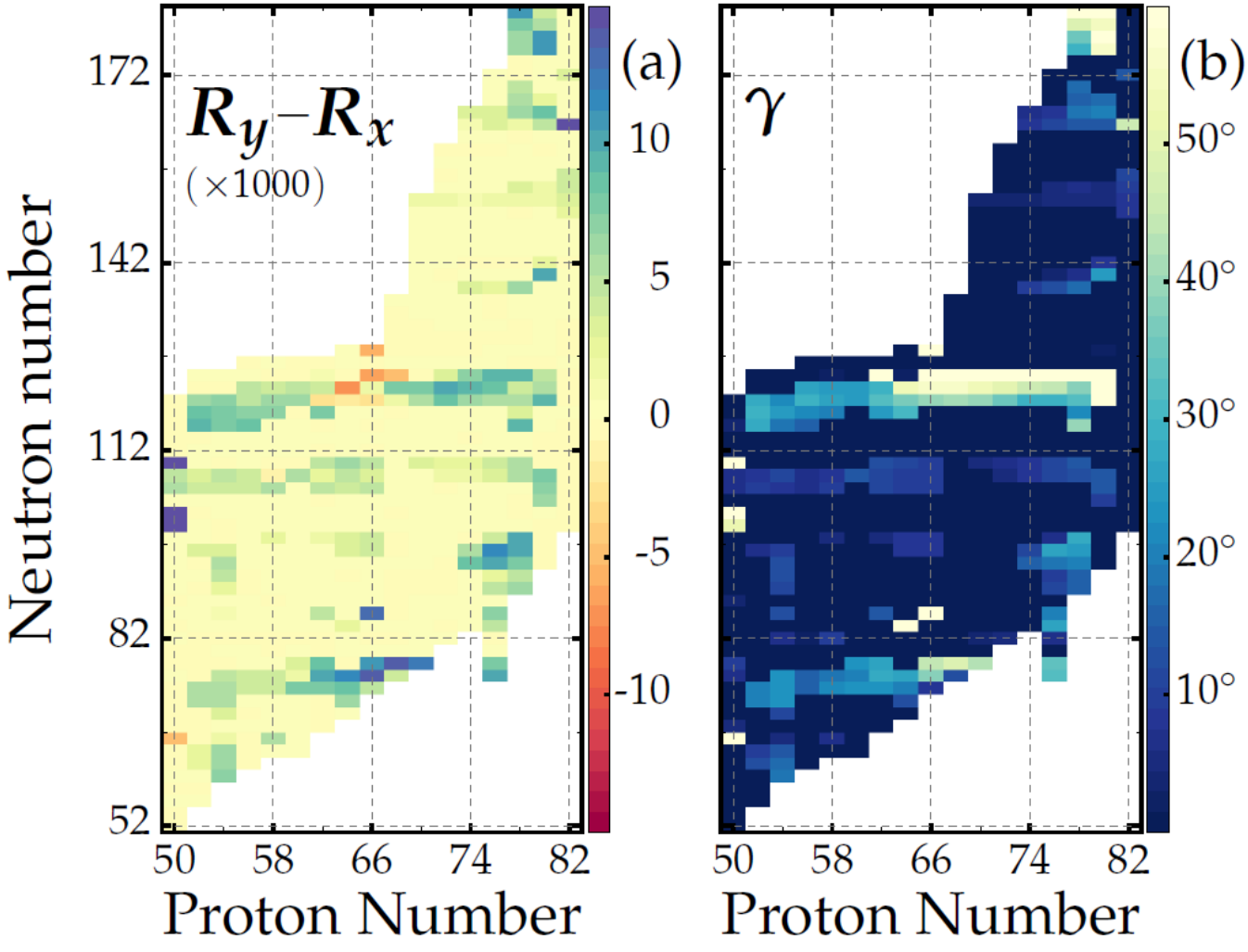
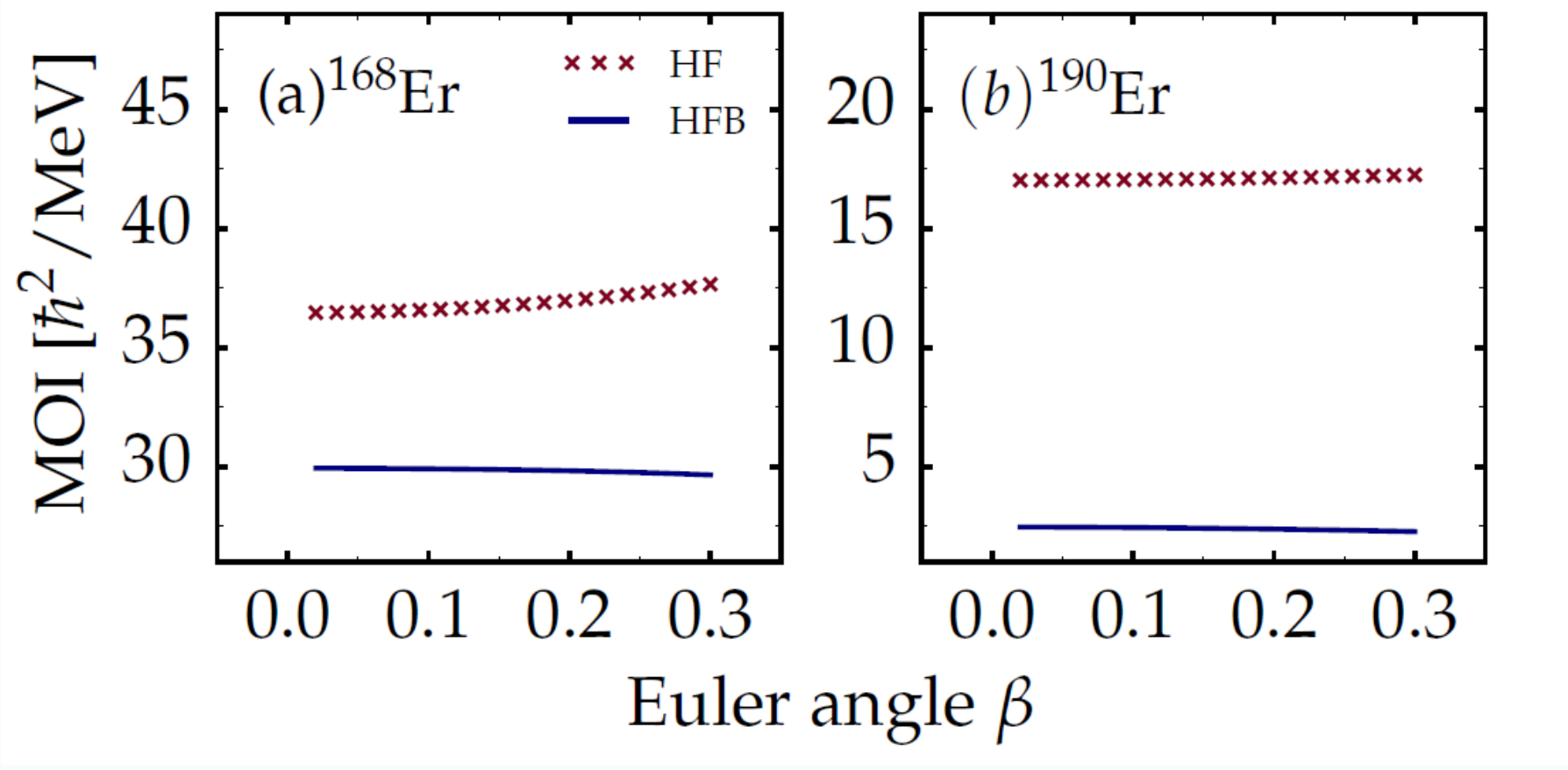


FIG. 4: (a) $R_y - R_x$: The difference between the mass ratios in the y- and x-directions. (b) Gamma deformations.

Y. Gao *et al.*, arXiv:1511.02814v2

Lipkin Moments of Inertia (MoI)



Y. Gao *et al.*, arXiv:1511.02814v2

We show results for the Lipkin parameters k re-represented in terms of the Lipkin Moments of Inertia (MoI) $\mathcal{J}$ as

$$\mathcal{J} \equiv \frac{1}{2k}.$$

Lipki MoI and energy corrections

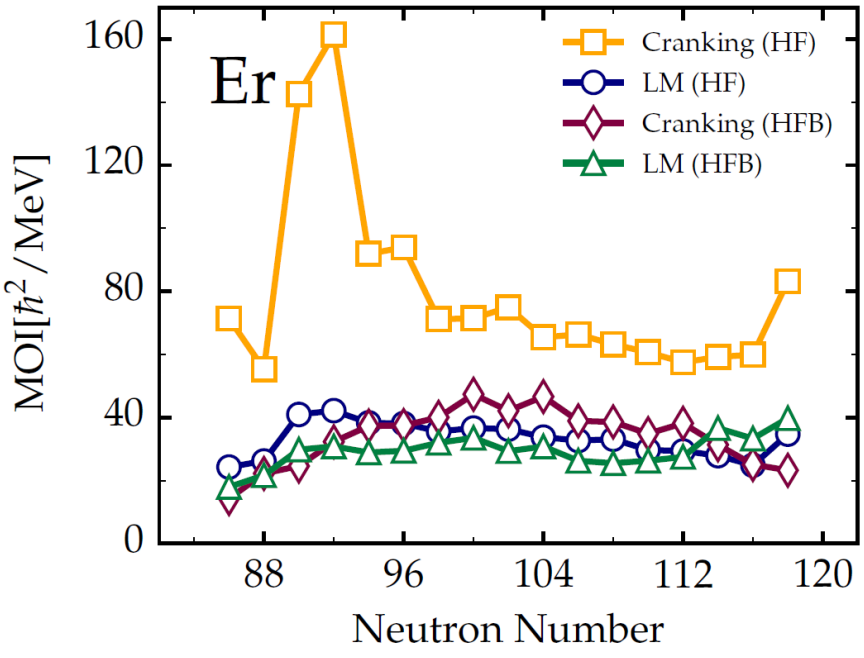


FIG. 10: MoI obtained using the Lipkin VAP method (LM) and cranking method with pairing correlations included (HFB) or not included (HF).

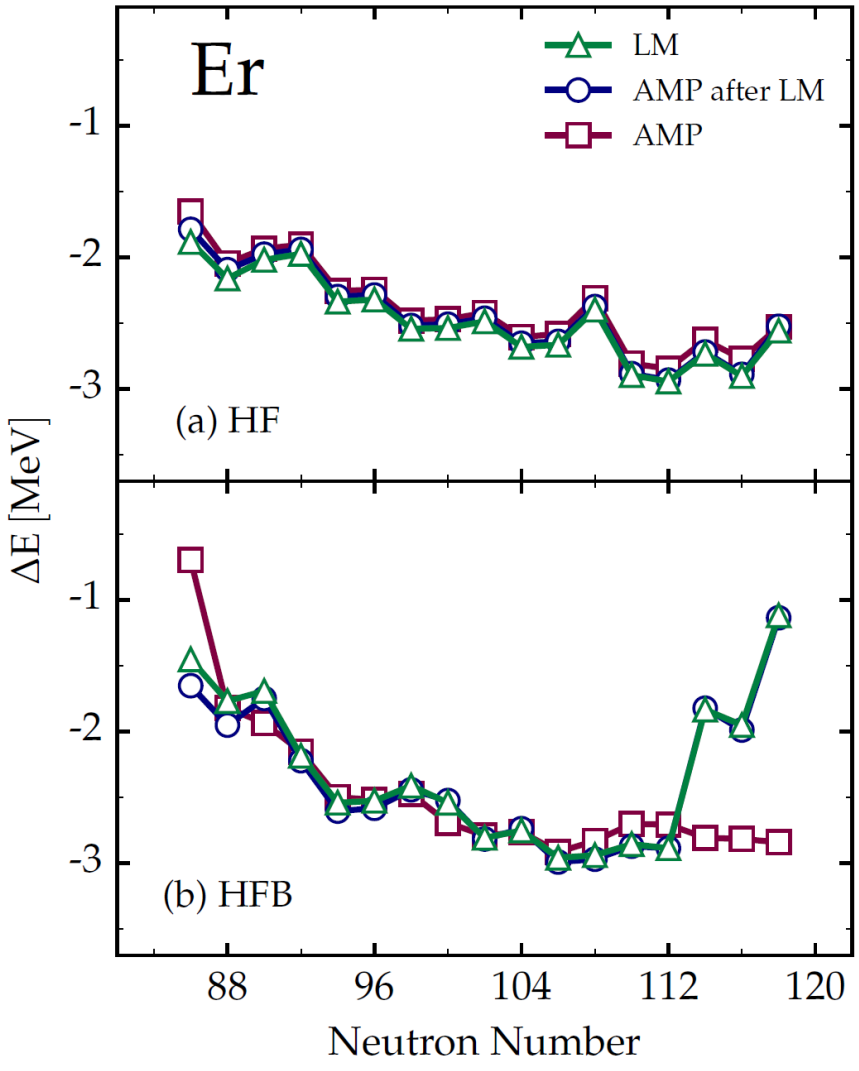


FIG. 7: Energy corrections obtained by the Lipkin VAP method (LM), AMP, and AMP after LM for erbium isotopes (a) without or (b) with pairing correlations.

Y. Gao *et al.*, arXiv:1511.02814v2

Thank you