A critical evaluation of the Gaussian Overlap Approximation (GOA)

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Outline

1. **Theoretical considerations**
2. **Center-of-mass motion**
3. **Rotation**
4. **Quadrupole deformation**
5. **(Open points)**

Theoretical considerations

- motivation of Gaussian Overlap Approximation (GOA)
- evaluation of GOA parameters in connection with energy-density functionals (EDF)

Generator Coordinate Method (GCM) in general

Path = set of mean-field states: $\{|\Phi_q\rangle\}$

Correlated state: $|\Phi\rangle = \int dq\,|\Phi_q\rangle\, f(q)$

Griffin-Hill-Wheeler (GHW) eq.: $\int dq'\, \mathcal{H}(q,q')\, f(q') = E \int dq'\, \mathcal{I}(q,q')\, f(q')$

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$\hat{H}$ unkown $\Longrightarrow$ $\mathcal{H}(q,q') = ??$ for $q \neq q'$

only the expectation value given: $\mathcal{H}(q,q'\!=\!q) \equiv E(\rho_q)\ ,\ \rho_q(r) = \langle\Phi_q|\hat{\rho}(r)|\Phi_q\rangle$

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Problems circumvented by the Gaussian Overlap Approximation (GOA)

$\Longrightarrow$ this talk: explore performance of (topological) GOA for typical collective motion

(ignoring here the further step to a collective Schrödinger equation)

The Gaussian Overlap Approximation (GOA)

Experience: overlaps qickly decreasing with $|q-q'|$ for fixed $\overline{q}=\dfrac{q+q'}{2}$

$\Longrightarrow$ approximate by Gaussians

$$\mathcal{I}(q,q') \approx \exp\left(\mathrm{i}\mu(q-q')-\frac{\lambda}{4}(q-q')^2\right)=\mathcal{I}^{(\mathrm{GOA})}(q,q')$$

$$\mathcal{H}(q,q') \approx \mathcal{I}^{(\mathrm{GOA})}(q,q')\left[\mathcal{H}_0(\overline{q})+\mathrm{i}(q-q')\mathcal{H}_1(\overline{q})-\frac{(q-q')^2}{8\lambda^2}\mathcal{H}_2(\overline{q})\right]$$

$$\lambda=2\langle\Phi_{\overline{q}}|\,\overleftarrow{\partial}_{\overline{q}}\overrightarrow{\partial}_{\overline{q}}\,|\Phi_{\overline{q}}\rangle \quad , \quad \mu=-\frac{\mathrm{i}}{2}\langle\Phi_{\overline{q}}|\,\overleftarrow{\partial}_{\overline{q}}-\overrightarrow{\partial}_{\overline{q}}\,|\Phi_{\overline{q}}\rangle$$

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GOA requires **collective** path $\leftrightarrow$ **many** s.p. states move each a **little** bit
simple example: *N*-boson state

$$\mathcal{I}(q,q') = (\langle\varphi_q|\varphi_{q'}\rangle)^N \approx \left[1-(q-q')\langle\varphi_{\overline{q}}|\overleftrightarrow{\partial}_{\overline{q}}|\varphi_{\overline{q}}\rangle-\frac{(q-q')^2}{2}\langle\varphi_{\overline{q}}|\overleftarrow{\partial}_{\overline{q}}\overrightarrow{\partial}_{\overline{q}}|\varphi_{\overline{q}}\rangle\right]^N$$

$$\approx \exp\left(\mathrm{i}\mu(q-q')-\frac{\lambda}{4}(q-q')^2\right)$$

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Advantage of GOA: $\mathcal{H}_0$ & $\mathcal{H}_2$ can be computed with EDF

$\mathcal{H}_0$: trivially as $\mathcal{H}_0=E(\rho_{\overline{q}})$ (expectation value of Slater state)

$\mathcal{H}_1$,$\mathcal{H}_2$: by analytical continuation (Wick rotation) $\rightarrow$ ...

Evaluation of $\mathcal{H}_2$ with EDF

define generating momentum: $\hat{P}|\Phi_q\rangle = \mathrm{i}\partial_q|\Phi_q\rangle$, $\langle\Phi_q|\hat{P} = -\mathrm{i}\langle\Phi_q|\partial_q$ (is a 1*ph* operator)

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$\mathcal{H}_2 = \langle\Phi_{\overline{q}}|\{\hat{P},\{\hat{H},\hat{P}\}\}|\Phi_{\overline{q}}\rangle$ = double anti-commutator - not yet suited for EDF

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rotate to imaginary q-axis $q \to -\mathrm{i}u$: (Wick rotation)

$$\Longrightarrow \quad |\tilde{\Phi}_u\rangle = \exp\left(u\hat{P}\right)|\Phi_0\rangle \ , \ \langle\tilde{\Phi}_u| = \langle\Phi_0|\exp\left(u\hat{P}\right)$$

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and $\langle\tilde{\Phi}_u|\hat{H}|\tilde{\Phi}_u\rangle \equiv E(\rho_u) \;,\; \rho_u(r) = \langle\Phi_u|\hat{\rho}(r)|\Phi_u\rangle$

$\Longrightarrow \quad \mathcal{H}_2 = \partial_u^2 E(\rho_u)|_{p=0}$ well defined in DFT

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$$\Longrightarrow \quad \mathcal{H}_2 = \partial_u^2 E(\rho_u)|_{p=0}$$ well defined in DFT

in principle applicable at any order $u^n \equiv$ analytical continuation

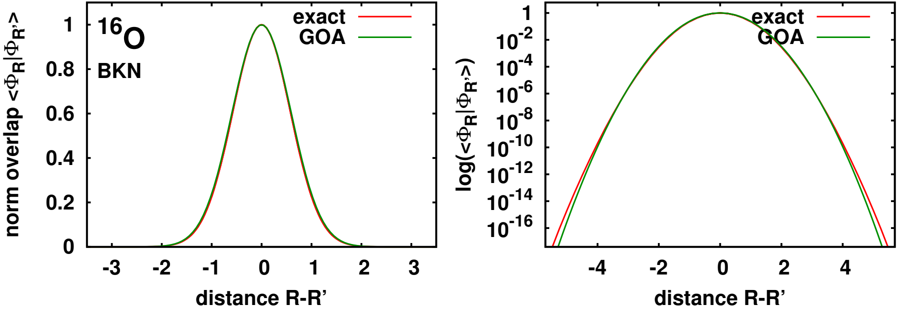
but the Taylor expansion has to exist – not guaranteed for most EDF

Center-of-mass motion

- quality of GOA for norm overlap of ^{16}O
- testing GOA for electro-magnetic formfactor of ^{16}O (quality depends on momentum q)
- counter example single-particle motion

GOA for c.m. motion

test case ^{16}O, SLy6 force
path: $|\Phi_R\rangle = \mathcal{A}\left\{\prod_\alpha \varphi_\alpha(r_\alpha - R)\right\}$ $\longleftrightarrow$ ideally collective



GOA is well satisfied

log plot reveals deviations in the far outside wings $\leftrightarrow$ correct asympt. $e^{-\gamma|R-R'|}$

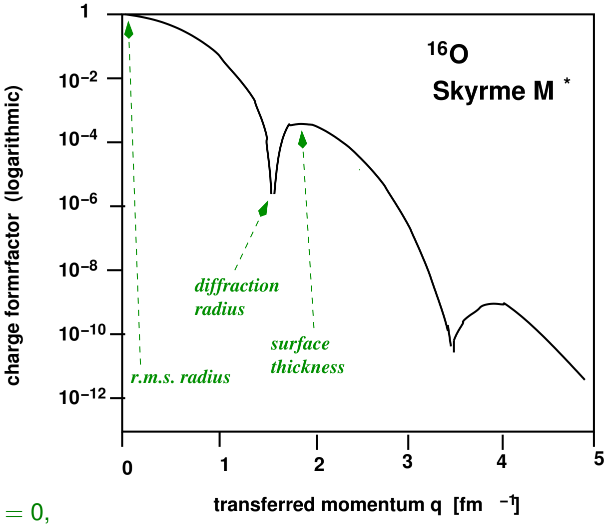
GOA well applicable for observables which concentrate on small $|R - R'|$

The nuclear formfactor

charge formfactor:

$F_C(\mathbf{q}) = \int d^3r\, e^{i\mathbf{q}\cdot\mathbf{r}} \rho_C(\mathbf{r})$

$\leftrightarrow$ electron scattering



r.m.s. radius $\leftrightarrow$ $\partial_q^2 F\Big|_{q=0}$,

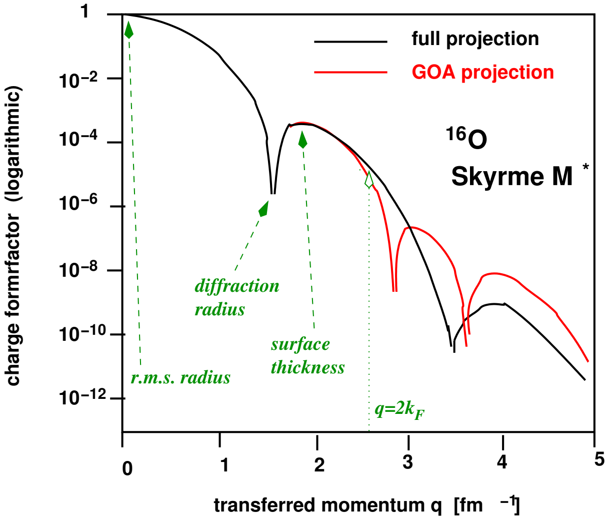
diffraction radius $\leftrightarrow$ $F(q^{(1)}) = 0$,

surface thickness $\leftrightarrow$ first maximum

Testing GOA for c.m. projection of the nuclear formfactor

projected state:

$$|\Psi\rangle = \int dR\, |\Phi_R\rangle$$



looks o.k. for $r_{\rm rms}$, $R_{\rm diffr}$, $\sigma_{\rm surf}$

quality depends on q:
large deviations for $q > 2k_{\rm F}$
($k_{\rm F}$ = Fermi momentum)

$q > 2k_{\rm F}$ anyway beyond mean-field description

GOA for c.m. projection more quantitatively

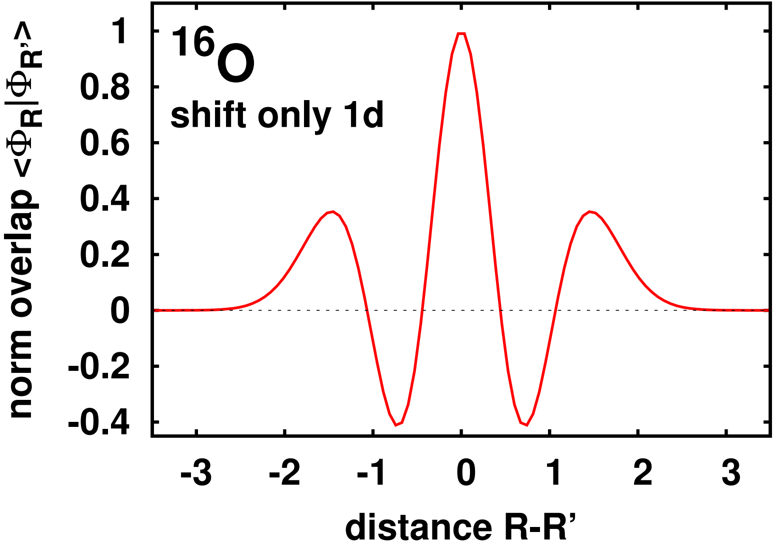
The difference between GOA and exact projection
for diffraction radius and surface thickness (computed with SkM*):

	^{12}C	^{16}O	^{40}Ca	^{48}Ca	^{208}Pb	present quality
$\delta R_{\rm diffr}$ [mfm]	35	-5	20	21	10	40
$\delta\sigma_{\rm surf}$ [mfm]	-30	-4	20	20	9	40

the effect on $r_{\rm rms}$ is negligible ($<$ 5 mfm)

$\Longrightarrow$ correction small compared to typical error on $R_{\rm diffr}$, $\sigma_{\rm surf}$
negligible for $A > 50$ – but beware when improving the precision

Counter example "non-collective": shift only $1d_{5/2,n}$ state in ^{17}O



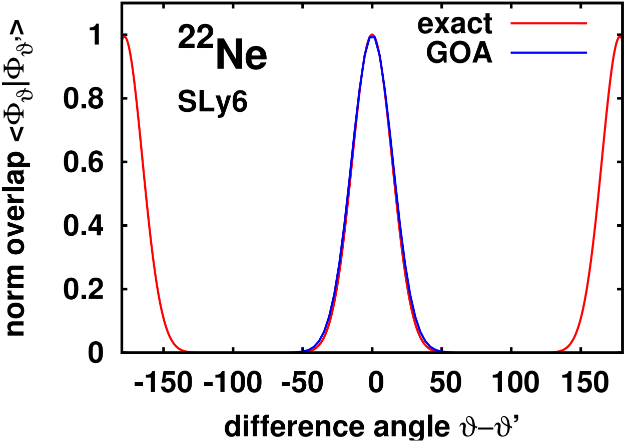
anything else than Gaussian – outcome unpredictable in simple terms

Rotation

- quality of GOA for norm overlap of ^{22}Ne
- extension to topologically augmented GOA (topGOA) for rotation
- counter example: rotation of ^{18}O (=single-particle motion)

GOA for rotation

test case ^{22}Ne, SLy6, path: $|\Phi_\vartheta\rangle = \exp\left(-\mathrm{i}\vartheta\hat{J}_y\right)|\Phi_0\rangle$



GOA is well satisfied in $-\pi < \vartheta < \pi$

but misses the basic structure of the exact $\mathcal{I}(\vartheta, \vartheta')$: π periodicity in $\vartheta - \vartheta'$

Topologically augmented GOA (topGOA) for rotation

GOA: $\mathcal{I}(q,q') \approx \exp\left(-\frac{\lambda}{4}(q-q')^2\right)$ for Cartesian coordinate $-\infty < q < +\infty$

but: rotation angle $-\pi \leq \vartheta \leq \pi$ and/or periodicity $\vartheta \longrightarrow \vartheta + 2\pi$

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$\Longrightarrow$ modify $q - q'$ to distance on the unit ring (sphere) $\sin(\vartheta - \vartheta')$:

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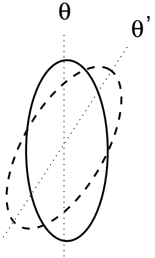

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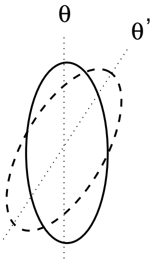

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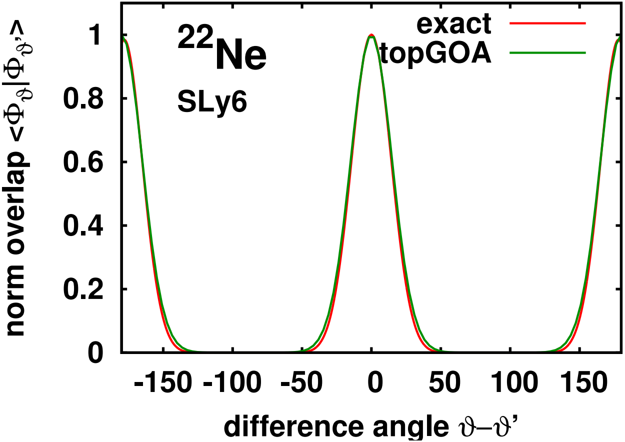
$$\mathcal{I}(q,q') \approx \exp\left(-\frac{\lambda}{4}\sin(\vartheta-\vartheta')^2\right)$$

and – take care of reflection symmetry = add reflected copy:

$$\mathcal{I}^{(\mathrm{topGOA})}(q,q') = \exp\left(-\frac{\lambda}{4}\sin(\vartheta-\vartheta')^2\right) + \exp\left(-\frac{\lambda}{4}\sin(\vartheta-\vartheta'+\pi)^2\right)$$

Topologically augmented GOA (topGOA) for rotation

test case ^{22}Ne, SLy6, path: $|\Phi_\vartheta\rangle = \exp\left(-\mathrm{i}\vartheta\hat{J}_y\right)|\Phi_0\rangle$



topGOA matches exact overlap very well (even for the small system ^{22}Ne)

Testing rotatonial topGOA for ^{18}O

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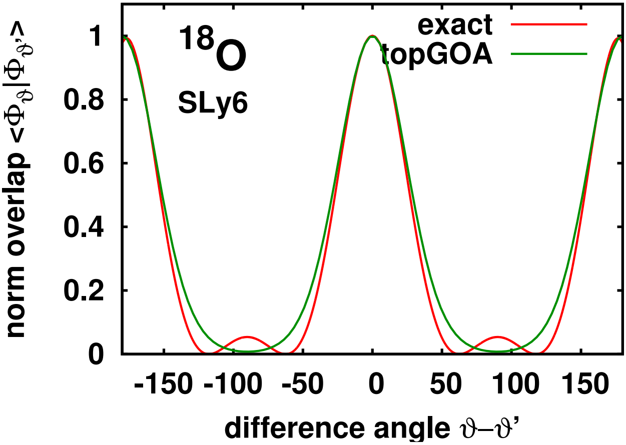

topGOA misses the extra peak at $\theta = \pm\pi/2$

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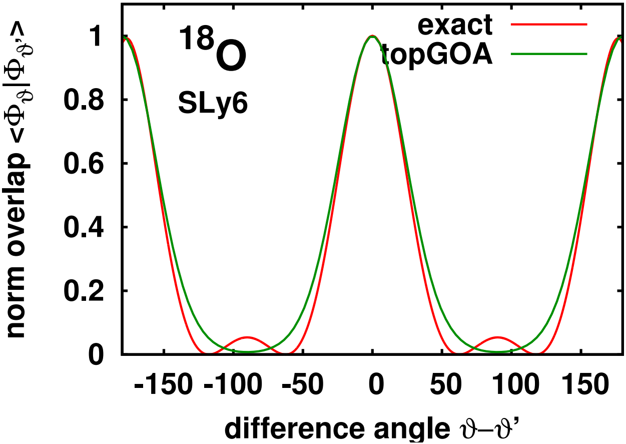
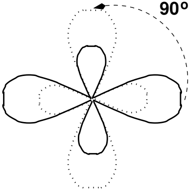


case not really collective dominated by one s.p. state
the neutron $1d_{5/2}$ state



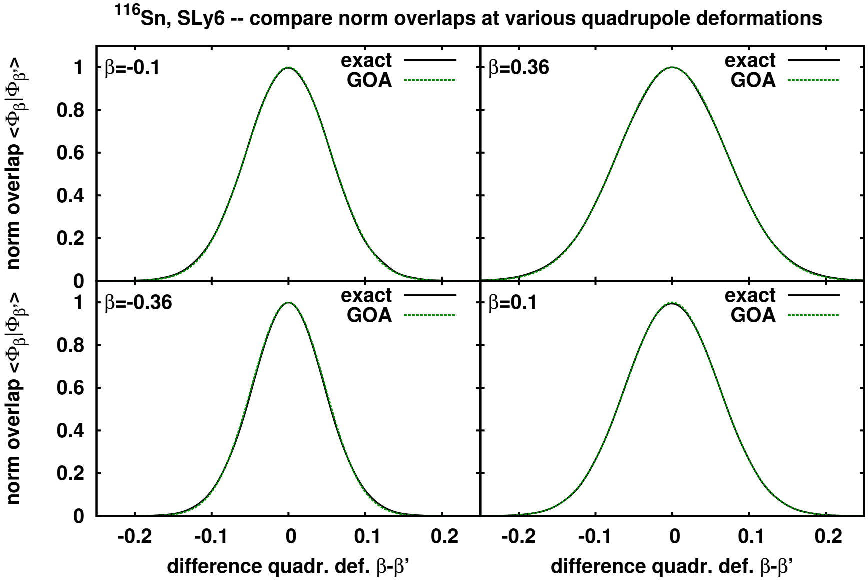
rotation by $\pi/2$
yields secondary peak

topGOA misses the extra peak at $\theta = \pm\pi/2$

Quadrupole deformation

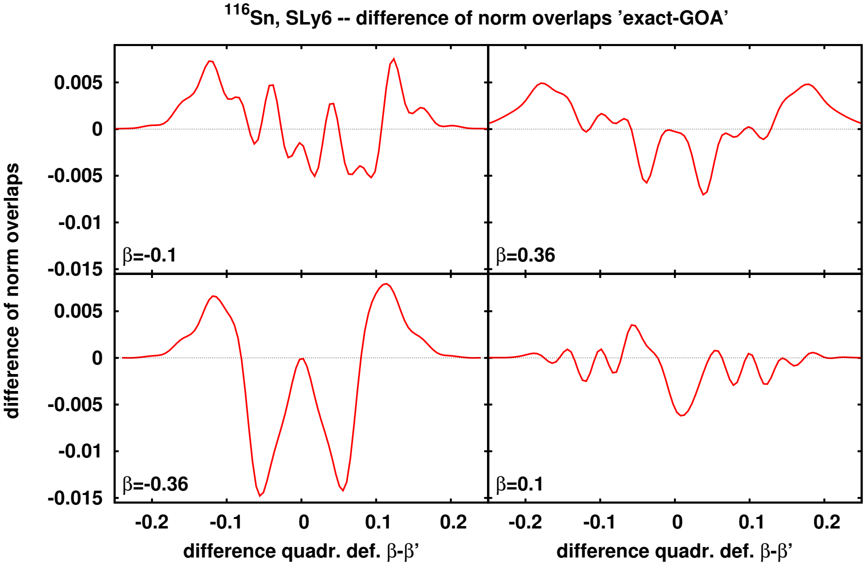
- testing GOA for norm overlap in ^{116}Sn
- testing GOA for norm overlaps along Sn chain
- testing GOA for collective kinetic energy along Sn chain
- collective $E(2_1^+)$ energies along Sn chain

GOA and exact overlap for quadrupole deformation in ^{116}Sn



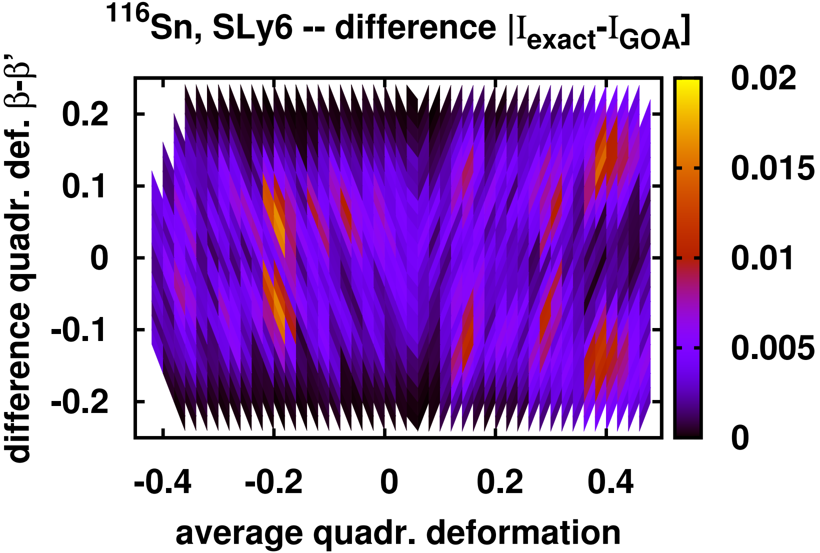
difference not really visible $\Longrightarrow$ amplify $\rightarrow$ ...

Diff. "GOA-exact" overlap for quadrupole deformation β in ^{116}Sn



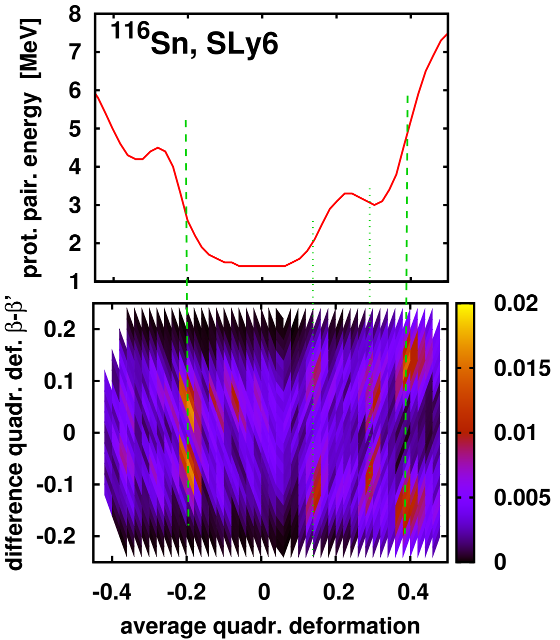
deviation depends on average deformation – but is very small everywhere

Map of diff. “GOA-exact” overlap for deformation β in ^{116}Sn



confirms results from previous snapshots: deviation is very small everywhere
regions of ”enhanced” deviation systematically at certain average deformations $\overline{\beta}$

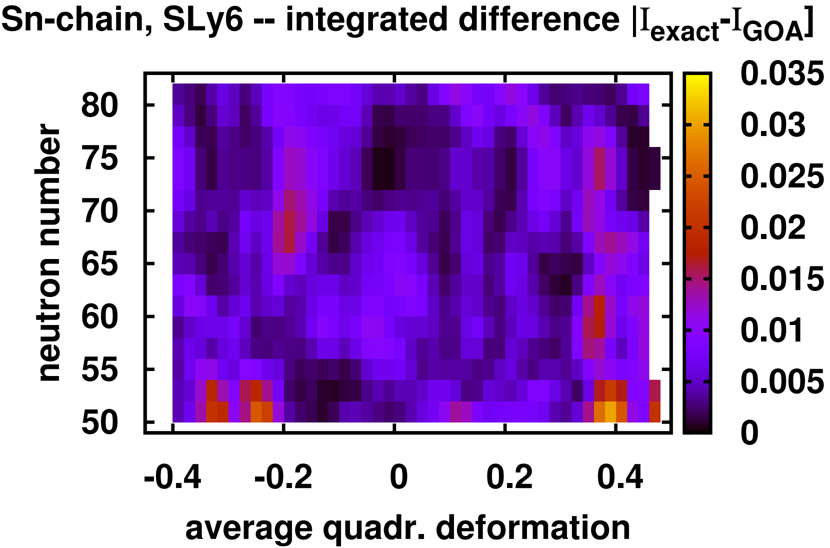
Compare map of diffences with proton pairing



regions of "enhanced" deviation are clearly correlated to regions of quickly changing pairing energy

(as indicated by green vertical lines)

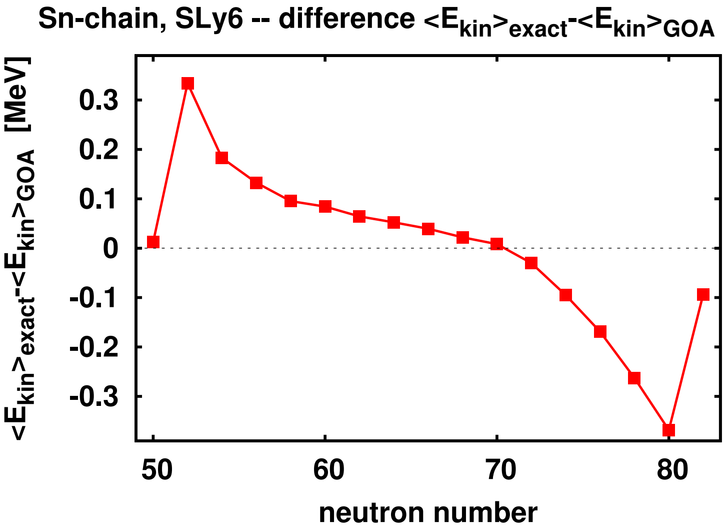
Average deviations along the chain of Sn isotopes



deviations remain small everywhere, have slight trend to grow for $N \searrow 50$

β regions with enhanced deviations are nearly independent of N

Difference “GOA-exact” for $\langle\Psi|\hat{T}|\Psi\rangle$ along Sn chain



acceptably small – as compared to typical 2_1^+ excitation energy ≈ 2 MeV
larger uncertainty next to shell closure ⟷ non-collective situation

Practical example: $E(2_1^+)$ energies in Sn and Pb chains

topGOA for vib.&rot. $\longrightarrow$ collective Schrödinger eq. in 5-dim. Bohr coordinates
(dynamical) path $\leftrightarrow$ axial CHF, linear response for vibration & rotation
interpolate potential, mass, inertia, GOA-width to triaxial plane

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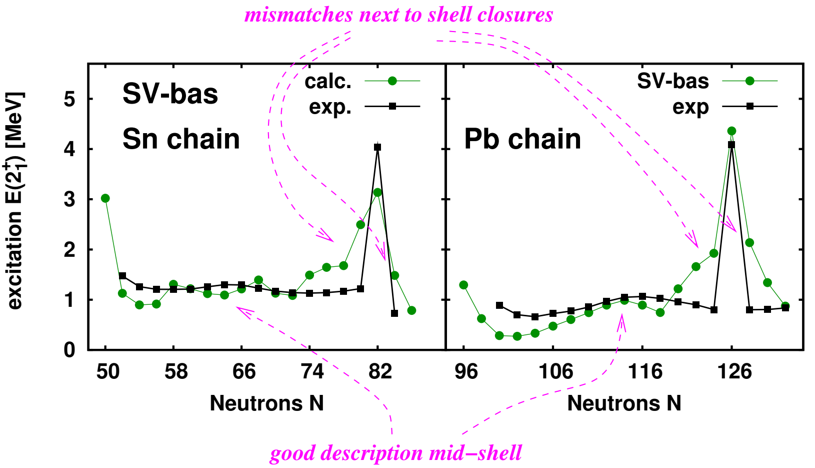
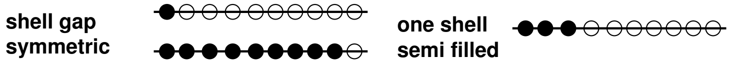


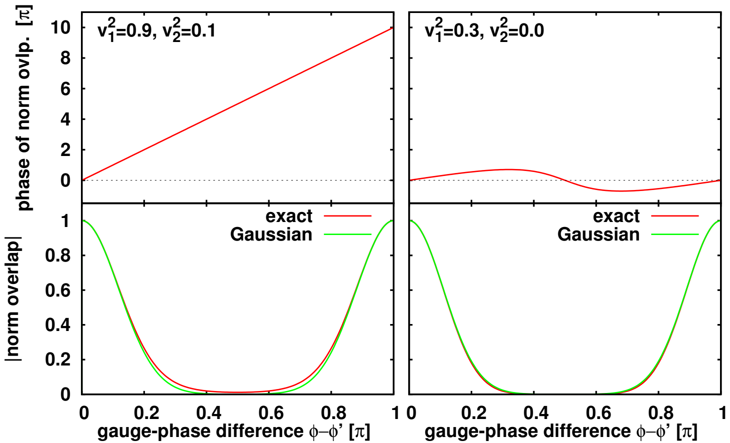
results comply with findings from study of error on collective kinetic energy
however: deviations near shell closures partly to to CHF instead of ATDHF

Open points in brief

Norm overlaps for gauge path (particle-number projection)

particle number projection $|\Psi\rangle = \int d\phi\, |\Phi_\phi\rangle$ $\leftrightarrow$ gauge path $|\Phi_\phi\rangle = e^{i\phi\hat{N}}|\Phi_0\rangle$





abs.value $|\mathcal{I}|$ could match GOA – but (complex) phase of $\mathcal{I}$ is changing regimes

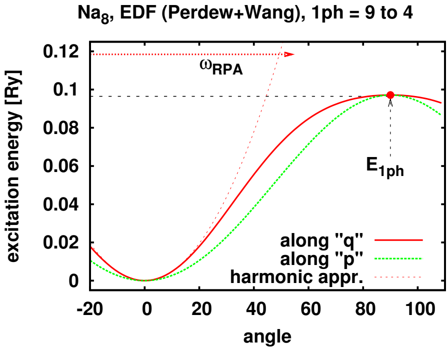
$1ph$ states: Discrepancy of EDF exp. value and RPA energy

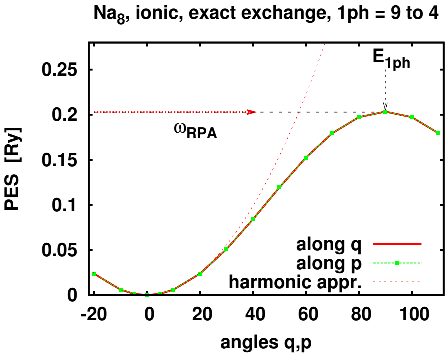
define generating operators: $\hat{P} = -\mathrm{i}(\hat{a}_p^\dagger \hat{a}_h - \text{h.c.})$, $\hat{Q} = \hat{a}_p^\dagger \hat{a}_h + \text{h.c.}$

$1ph$ path: $|\Phi_{qp}\rangle = \exp\left(\mathrm{i}p\hat{Q}\right)\exp\left(-\mathrm{i}q\hat{P}\right)|\Phi_0\rangle$, limiting case, e.g., $|\Phi_{\pi/2,0}\rangle = \hat{a}_p^\dagger \hat{a}_h |\Phi_0\rangle$

"RPA"=small oscillations along $qp \Rightarrow \omega_{\mathrm{RPA}} \longleftrightarrow$ direct EDF evaluation $E_{ph} = E_{\mathrm{EDF}}[\rho_{ph}]$

test case is an electronic system: Na_8 cluster with P&W EDF compared to exact exchange





results perfectly consistent for exact exchange – but dramatic difference for EDF

Conclusions

Formal aspects

$\langle\Phi_q|\hat{H}|\Phi_{q'}\rangle$ not given in DFT, may be recovered by analytical continuation
problems with non-analiticity of energy-density functionals
GOA complies with DFT $\leftrightarrow$ only lowest order Wick rotation
GOA implies collective deformations

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Realistic test cases

center-of-mass	ideally collective, works fine for bulk observables
	fails for high momenta (small distances)
rotation	requires topological extension $\longrightarrow$ topGOA
	works fine for collective rotation (^{22}Ne), fails for s.p. structures (^{18}O)
quadrupole	quality varies along the path (beware of quickly changing pairing)
	typical uncertainty on collective excitation energies $\approx$ 0.2 MeV
	more uncertainty next to magic shells (s.p. structures)

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Future developments

GOA may be improved by extending Wick rotation to 4. order
EDF directly for $\langle\Phi_q|\hat{H}|\Phi_{q'}\rangle$

Appendix: additional material in reserve

Non-diagonal overlaps by analytical continuation

for simplicity set $\overline{q}=0$, thus considering

$$\begin{aligned}\mathcal{H}(q) &= \langle\Phi_{-q}|\hat{H}|\Phi_q\rangle = \langle\Phi_0|e^{-\mathrm{i}q\hat{P}}\hat{H}e^{-\mathrm{i}q\hat{P}}|\Phi_0\rangle \equiv \langle e^{-\mathrm{i}q\hat{P}}\hat{H}e^{-\mathrm{i}q\hat{P}}\rangle \\ &= \langle\hat{H}\rangle - \mathrm{i}q\langle\{\hat{H},\hat{P}\}\rangle - \frac{q^2}{2}\langle\{\{\hat{H},\hat{P}\},\hat{P}\}\rangle + \mathrm{i}\frac{q^3}{6}\langle\{..\hat{H},\underbrace{..\hat{P}\}}_{3}\rangle + \frac{q^4}{24}\langle\{..\hat{H},\underbrace{..\hat{P}\}}_{4}\rangle...\end{aligned}$$

turn to purely imaginary coordinate $q\longrightarrow\mathrm{i}u \quad\Longrightarrow\quad |\tilde{\Phi}_u\rangle = e^{u\hat{P}}|\Phi_0\rangle \quad\Longrightarrow$

$$\begin{aligned}\tilde{\mathcal{H}}(u) &= \langle\Phi_u|\hat{H}|\Phi_u\rangle = \\ &= \langle\hat{H}\rangle + u\langle\{\hat{H},\hat{P}\}\rangle + \frac{u^2}{2}\langle\{\{\hat{H},\hat{P}\},\hat{P}\}\rangle + \frac{u^3}{6}\langle\{..\hat{H},\underbrace{..\hat{P}\}}_{3}\rangle + \frac{u^4}{24}\langle\{..\hat{H},\underbrace{..\hat{P}\}}_{4}\rangle...\end{aligned}$$

DFT identification as $\tilde{\mathcal{H}}(u)=E(\rho_u)\Rightarrow$ reconstruct $\mathcal{H}(q)$ by analytical continuation

e.g. by identifying $\partial_u^n\tilde{\mathcal{H}}=(-I)^n\partial_q^n\mathcal{H}$

problem: $\tilde{\mathcal{H}}(u)$ has to be analytical (Taylor expandable) $\longleftrightarrow$ usually not provided

GOA requires only existence up to q^2 (u^2) $\longleftrightarrow$ usually possible

hope: stepwise improvement of GOA by going to higher order, e.g., q^4

TopGOA in the 5-dimensional quadrupole plane

Cartesian $\alpha_{2\mu}, \mu=-2,...,+2 \quad \longleftrightarrow \quad$ intrinsic (Bohr) $(\beta,\gamma,\vartheta_x,\vartheta_y,\vartheta_z)$

$$\alpha_{2\mu}(\beta,\gamma,\boldsymbol{\vartheta}) \quad = \quad \beta\left[\cos\gamma D^{(2)}_{\mu 0}(\boldsymbol{\vartheta}) + \sin\gamma\frac{D^{(2)}_{\mu +2}(\boldsymbol{\vartheta}) + D^{(2)}_{\mu -2}(\boldsymbol{\vartheta})}{2}\right]$$

GOA appropriate for Cartesian coord.: $\mathcal{I}^{(\mathrm{Cart})}(\boldsymbol{\alpha},\boldsymbol{\alpha}') = e^{-\frac{1}{4}(\alpha_\mu-\alpha'_\mu)^*\lambda_{\mu\nu}(\alpha_\nu-\alpha'_\nu)}$

topGOA for Bohr coordinates by transformation of $\mathcal{I}^{(\mathrm{Cart})}$:

1) insert $\alpha_{2\mu} = \alpha_{2\mu}(\beta,\gamma,\boldsymbol{\vartheta})$

2) transform width matrix $\lambda_{\mu\nu}$ to intrinsic $\lambda^{\mathrm{intr}}_{ij}$

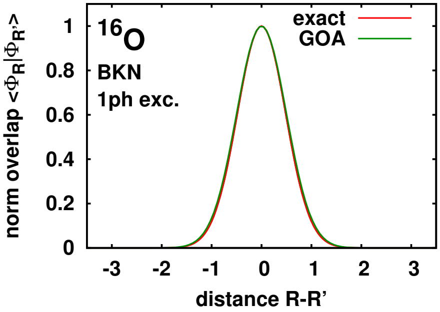
$$\begin{aligned} \lambda_{\mu\nu} &= W_i^\mu \lambda^{\mathrm{intr}}_{ij} W_j^\nu \\ W_i^\mu &: \quad \nabla_i = W_i^\mu \nabla_{\alpha_{2\mu}} \quad , \quad i \in \{\beta,\gamma,\boldsymbol{\vartheta}\} \end{aligned}$$

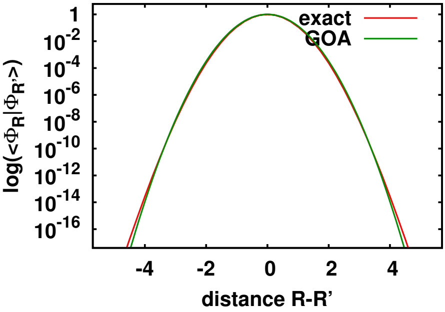
3) exploit symmetries $\quad \lambda^{\mathrm{intr}}_{ij} = \begin{pmatrix} \lambda_{\beta\beta} & \lambda_{\beta\gamma} & 0 & 0 & 0 \\ \lambda_{\gamma\beta} & \lambda_{\gamma\gamma} & 0 & 0 & 0 \\ 0 & 0 & \lambda_x & 0 & 0 \\ 0 & 0 & 0 & \lambda_y & 0 \\ 0 & 0 & 0 & 0 & \lambda_z \end{pmatrix}$

practically: evaluate by Maple, feed in directly to Fortran code

GOA for c.m. motion – excited state

test case ^{16}O, BKN force
consider path built on excited state $\hat{a}^\dagger_{1d_{5/2}}\hat{a}_{1p_{1/2}}|\Phi\rangle$





GOA is also well satisfied for this case

$\Longrightarrow$ c.m. motion is most robust