Multi-reference Energy Density Functional calculations for nuclei

Constraints from consistency requirements

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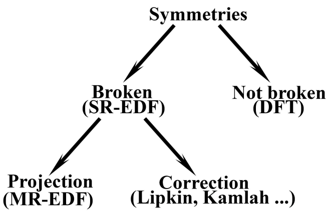
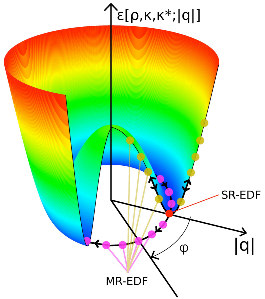
Outline

Talk in one slide

Context

1. Two-step nuclear EDF method (i) single-reference (ii) multi-reference
2. Built by analogy with wave-function based methods (no existence theorem)
3. SR-EDF has both similarities and differences with (standard) DFT
4. Strongly relies on spontaneous symmetry breaking and restoration





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Take-away message

1. MR-EDF tackles long-range correlations and accesses collective excitations
2. QRPA is recovered from the harmonic limit of MR-EDF
3. MR-EDF calculations must be constrained through consistency requirements

Outline

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Ingredients of the nuclear EDF method

Two-level variational wave-function method

1^{st} **level: HFB**	2^{nd} **level: projected HFB + GCM**
Trial WF: $\vert\Phi_q\rangle = \prod_\mu \beta^q_\mu \vert 0\rangle$	Trial WF: $\vert\Psi\rangle = \sum_q f_q \vert\Phi_q\rangle = \sum_{\vert q\vert} g_{\vert q\vert} P_X \vert\Phi_{\vert q\vert}\rangle$
Sym. break. $q = \vert q\vert e^{i\varphi} \neq 0$	Sym. restor. $(\sum_\varphi)$ and zero-point fluct. $(\sum_{\vert q\vert})$

$$[\mathbf{X},\mathbf{H}] = \mathbf{0} \text{ for } \{\mathbf{X}\} = \{\mathbf{N},\mathbf{Z},\mathbf{P},\mathbf{J^2},\mathbf{J_z},\mathbf{T^2},\mathbf{T_z},\mathcal{T}^\mathbf{2}\}$$

Static collective correlations	*Dynamical* collective correlations
$E^{1^{\text{st}}}_{\vert q\vert} = \langle\Phi_q\vert H\vert\Phi_q\rangle$ $\Downarrow$ Standard Wick Theorem $\Downarrow$ $\langle\Phi_q\vert H\vert\Phi_q\rangle = E[\rho^{qq},\kappa^{qq},\kappa^{qq\,*}]$	$E^{2^{\text{nd}}}_X = \langle\Psi\vert H\vert\Psi\rangle = \sum_{qq'} f^*_q f_{q'} \langle\Phi_q\vert H\vert\Phi_{q'}\rangle$ $\Downarrow$ Generalized Wick Theorem $\Downarrow$ $\langle\Phi_q\vert H\vert\Phi_{q'}\rangle = E[\rho^{qq'},\kappa^{qq'},\kappa^{q'q\,*}]\,\langle\Phi_q\vert\Phi_{q'}\rangle$
$\mathbf{E^{1^{st}}_{\vert q\vert}}$ **is a functional of** *diagonal* **density matrices** $\rho^{\mathbf{qq}},\kappa^{\mathbf{qq}}$ and $\kappa^{\mathbf{qq}\,*}$	$\mathbf{E^{2^{nd}}_X}$ **invokes the SAME functional of (all)** *transition* **density matrices** $\rho^{\mathbf{qq'}},\kappa^{\mathbf{qq'}}$ and $\kappa^{\mathbf{q'q}\,*}$

Ingredients of the nuclear EDF method

Two-level energy density functional method

1^{st} **level: single-reference**	2^{nd} **level: multi-reference**
Trial state $\vert\Phi_q\rangle = \prod_\mu \beta_\mu^q \vert 0\rangle$	Trial **set of states** $\{\vert\Phi_q\rangle\} \neq \vert\Psi\rangle$
Sym. break. $q = \vert q\vert e^{i\varphi} \neq 0$	Sym. restor. $(\sum_\varphi)$ and zero-point fluct. $(\sum_{\vert q\vert})$

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Static collective correlations	Dynamical collective correlations
$\mathcal{E}^{\text{SR}}_{\vert q\vert} \equiv \mathcal{E}[\Phi_q;\Phi_q]$	$\mathcal{E}^{\text{MR}}_X \equiv \sum_{qq'} f_q^* f_{q'}\, \mathcal{E}[\Phi_q;\Phi_{q'}]\, \langle\Phi_q\vert\Phi_{q'}\rangle \neq \langle\Psi\vert H\vert\Psi\rangle$

Bulk of correlations resummed into $\mathcal{E}[\Phi_q;\Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q*}]$

$\delta\left[\mathcal{E}^{\text{SR}} - \lambda\text{Tr}\{\rho\} - \lambda^{\vert\mathbf{q}\vert}\text{Tr}\{\rho\mathbf{Q}\}\right] = \mathbf{0}$ $\Downarrow$ **HFB-like equations**	$\delta\mathcal{E}^{\text{MR}}_{\mathbf{X}}/\delta\mathbf{f}^*_{\mathbf{q}} = \mathbf{0}$ $\Downarrow$ **Hill-Wheeler-Griffin-like equations**

Ingredients of the nuclear EDF method

Two-level energy density functional method

1^{st} level: single-reference	2^{nd} level: multi-reference
Trial state $\vert\Phi_q\rangle = \prod_\mu \beta_\mu^q \vert 0\rangle$	Trial **set of states** $\{\vert\Phi_q\rangle\} \neq \vert\Psi\rangle$
Sym. break. $q = \vert q\vert e^{i\varphi} \neq 0$	Sym. restor. $(\sum_\varphi)$ and zero-point fluct. $(\sum_{\vert q\vert})$

Relevant questions

1. Is the WF→EDF mapping efficient? Is it safe? How is it constrained?
2. Is the GWT-inspired mapping $\mathcal{E}[\Phi_q;\Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q*}]$ appropriate?
3. What is the connection of all that to QRPA?
4. What is the link to (Ensemble) DFT?

Bulk of correlations resummed into $\mathcal{E}[\Phi_q;\Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q*}]$

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$\Downarrow$	$\Downarrow$
HFB-like equations	**Hill-Wheeler-Griffin-like equations**

Outline

Ground-state correlation energy associated with $X = J^2$

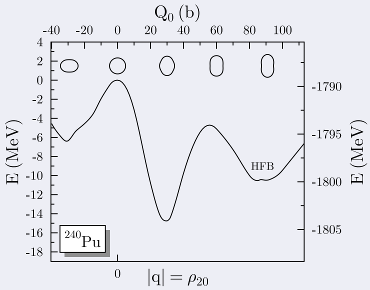
Collective coordinates = "Order parameter"

1. $|q|$ = multipole moments of $\rho(\vec{r})$
2. φ = Euler angles (α, β, γ)

From static deformation

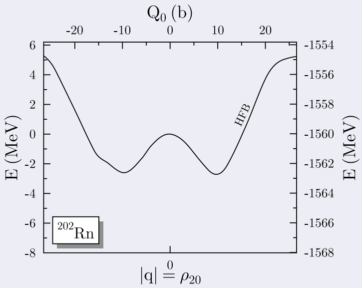
$$\Delta\mathcal{E}^{\text{SR}}_{|q|_{\text{min}}} = \text{Min}_{|q|}\left\{\mathcal{E}^{\text{SR}}_{|q|}\right\} - \mathcal{E}^{\text{SR}}_{0}$$

Well-deformed nucleus for $|q| = \rho_{20}$



[M. Bender, private communication]

Transitional nucleus for $|q| = \rho_{20}$



[M. Bender, private communication]

Ground-state correlation energy associated with $X = J^2$

Collective coordinates = "Order parameter"

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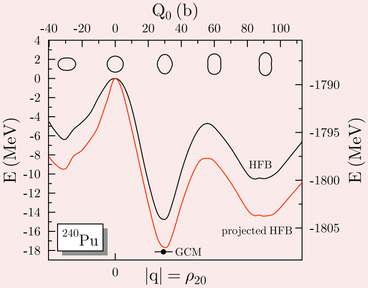
From dynamical fluctuations

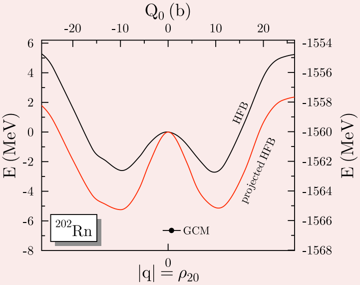
$$\Delta\mathcal{E}^{\text{MR}}_{J=0} = \mathcal{E}^{\text{MR}}_{J=0} - \text{Min}_{|q|}\left\{\mathcal{E}^{\text{SR}}_{|q|}\right\}$$

Stiff nucleus for $|q| = \rho_{20}$



[M. Bender, private communication]

Soft nucleus for $|q| = \rho_{20}$

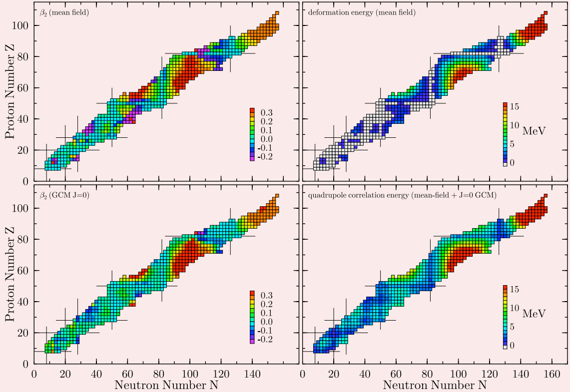


[M. Bender, private communication]

Ground-state correlation energy associated with $X = J^2$

Systematic of quadrupole correlations: $\rho_{20} \neq 0 + J = 0 + \Delta\rho_{20}$

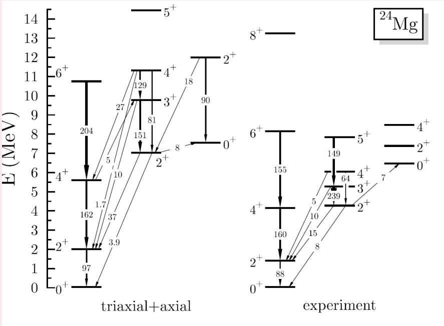
[M. Bender, G.-F. Bertsch, P.-H. Heenen, PRC73 (2006) 034322]



1. Deformation/fluctuations dominant in heavy/light nuclei
2. Right balance between open- and closed-shell nuclei from single EDF
3. Improve ground-state observables systematically, e.g. $\sigma^{\mathrm{mass}}_{2149} = 800\mathrm{keV}$

Collective excitations

Restoration of $N, Z, J^2, M + \Delta\rho_{20} + \Delta\rho_{22}$



[M. Bender, P.-H. Heenen, PRC78 (2008) 024309]

Energy spectrum

- Vibrational + rotational states
- Nicely aligned with experiment
- Too spread out spectrum

Electromagnetic transitions

- Restoration of (J^2, J_z) essential
- Selection rules recovered
- Good in- and out-band $B(E2)$

Outline

Link with QRPA

QRPA from Time-Dependent SR-EDF calculations

1. Adiabatic-type scheme (omitting anomalous densities κ)

$$A_{minj} = (\epsilon_m - \epsilon_i)\,\delta_{mn}\,\delta_{ij} + \frac{\partial^2 \mathcal{E}[\rho]}{\partial\rho_{im}\partial\rho_{nj}} \quad ; \quad B_{minj} = \frac{\partial^2 \mathcal{E}[\rho]}{\partial\rho_{im}\partial\rho_{jn}}$$

2. Extensions (e.g. second RPA...) needed to access *spreading width*

QRPA from Projection+GCM in WF method

- QRPA (WF)

$$A_{minj} = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \bar{v}_{mjin} \quad ; \quad B_{minj} = \bar{v}_{mnij}$$

- QRPA (WF) is recovered from the harmonic limit of GCM (WF) [B. Jancovici, D. H. Schiff, NP58 (1964) 678]
  1. Use Thouless parameterization $|\Phi_q\rangle = \exp[\sum_{im} z^{q*}_{mi} a^\dagger_m a_i]|\Phi_0\rangle$
  2. Expand $\langle\Phi_q|H|\Phi_{q'}\rangle/\langle\Phi_q|\Phi_{q'}\rangle$ to second order in $\mathbf{z^q}/\mathbf{z^{q'}}^*$
  3. Assume gaussian overlap $\langle\Phi_q|\Phi_{q'}\rangle \propto \exp[\mathrm{Tr}(\mathbf{z^q}\mathbf{z^{q'}}^\dagger)]$
- HFB + GCM can tackle large amplitude *anharmonic* collective motions

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Set of constraints from consistency requirements

SR-EDF [J. Dobaczewski, J. Dudek, APP B27 (1996) 45]

- $\mathcal{E}^{SR}_{|q|}$ must be real and a scalar under all $\mathcal{R}(g) \in$ symmetry group $\mathcal{G}$
- Rules to build local Skyrme EDF to 2^{nd} order in σ_ν and ∇

$$\mathcal{E}[\rho,\kappa,\kappa^*] \equiv \int d\vec{r}\,\mathcal{E}[\rho_T(\vec{r}),\tau_T(\vec{r}),J_{T,\mu\nu}(\vec{r}),\vec{s}_T(\vec{r}),\vec{j}_T(\vec{r}),\vec{T}_T(\vec{r}),\vec{F}_T(\vec{r}),\tilde{\rho}_T(\vec{r});\nabla]$$

MR-EDF [L. Robledo, IJMP E16 (2007) 337; JPG: Nucl. Part. Phys. 37 (2010) in press]

1. $\mathcal{E}^{MR}_{X}$ must be real and a scalar under all $\mathcal{R}(g) \in$ symmetry group $\mathcal{G}$
2. Consistency of MR and SR schemes
   1. $\mathcal{E}^{MR}_{X} = \mathcal{E}^{SR}_{|q|}$ when $\{|\Phi_q\rangle\} \longrightarrow |\Phi_q\rangle$
   2. Chemical potential λ must be recovered from Kamlah expansion of $\mathcal{E}^{MR}_{N}$
   3. QRPA must be recovered through harmonic limit of $\mathcal{E}^{MR}_{X}$

Extension to MR kernel must implicate *transition* densities only

Diagonal SR kernel		**Off-diagonal MR kernel**
$\mathcal{E}[\rho^{\mathbf{qq}},\kappa^{\mathbf{qq}},\kappa^{\mathbf{qq}*}]$	GWT-inspired connection (only) viable option?	$\mathcal{E}[\rho^{\mathbf{qq}'},\kappa^{\mathbf{qq}'},\kappa^{\mathbf{q}'\mathbf{q}*}]$

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Outline

Unexpected pathologies

The example of particle number restoration (PNR)

- MR set $\{|\Phi_\varphi\rangle \equiv e^{i\hat{N}\varphi}|\Phi_0\rangle\,;\, \varphi \in [0, 2\pi]\}$
- Real, scalar, particle-number-restored MR energy reads

$$\mathcal{E}_N^{MR} \equiv \int_0^{2\pi} d\varphi\, \frac{e^{-i\varphi N}}{2\pi\, c_N^2}\, \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]\, \langle \Phi_0 | \Phi_\varphi \rangle$$

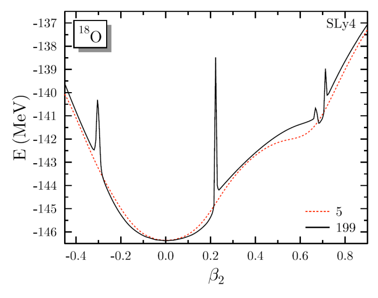
that corresponds to the Fourier decomposition of MR kernel on $U(1)$ Irreps

$$\begin{aligned} \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]\, \langle \Phi_0 | \Phi_\varphi \rangle &= \sum_{N\in\mathbb{Z}} c_N^2\, \mathcal{E}_N^{MR}\, e^{iN\varphi} \\ \langle \Phi_0 | \Phi_\varphi \rangle &= \sum_{N\in\mathbb{Z}} c_N^2\, e^{iN\varphi} \end{aligned}$$

- So far so good...

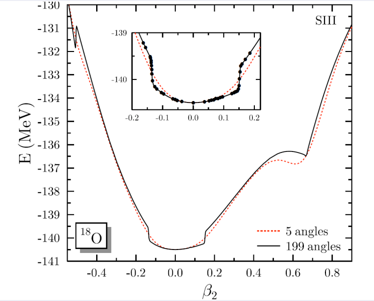
Unexpected pathologies

$\mathcal{E}^{MR}_{Z=8,N=10}$ vs ρ_{20} for $\mathcal{E}[\rho\rho\rho^{1/6}]$



[M. Bender *et al.*, PRC79 (2009) 044319]

$\mathcal{E}^{MR}_{Z=8,N=10}$ vs ρ_{20} for $\mathcal{E}[\rho\rho\rho]$



[M. Bender *et al.*, PRC79 (2009) 044319]

1. Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
2. Non-analyticity of $\mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]$ over $\mathbb{C}$-plane with $e^{i\varphi} \equiv z$
3. $\mathcal{E}^{MR}_{N} \neq 0$ for $N \leq 0$!! [M. Bender, T.D., D. Lacroix, PRC79 (2009) 044319]
4. Similar problems for other MR modes, e.g. angular momentum restoration

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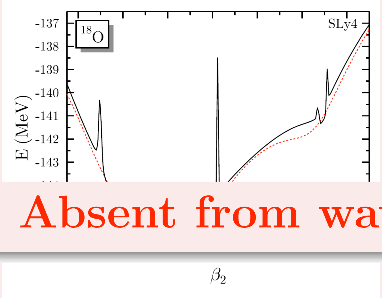

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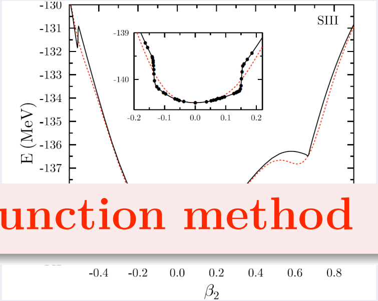

[M. Bender *et al.*, PRC79 (2009) 044319]

Absent from wave-function method

1. Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
2. Non-analyticity of $\mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]$ over $\mathbb{C}^*$ via $e^{i\varphi} \equiv z$
3. $\mathcal{E}^{MR}_N \neq 0$ for $N \leq 0$!! [M. Bender, T.D., D. Lacroix, PRC79 (2009) 044319]
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Outline

Regularization method

Origin of the problem and its solution

- Alternative method to define $\mathcal{E}[\Phi_q;\Phi_{q'}]$ that relies on
  1. Considering Bogoliubov transformation connecting $|\Phi_q\rangle$ to $|\Phi_{q'}\rangle$
  2. Using Bloch-Messiah-Zumino decomposition to reach BCS-like connection

$$|\Phi_{q'}\rangle = \tilde{\mathcal{C}}_{qq'} \prod_{p>0} \left(\bar{A}^*_{pp} + \bar{B}^*_{p\bar{p}}\, \tilde{\alpha}^+_p\, \tilde{\alpha}^+_{\bar{p}}\right) |\Phi_q\rangle$$

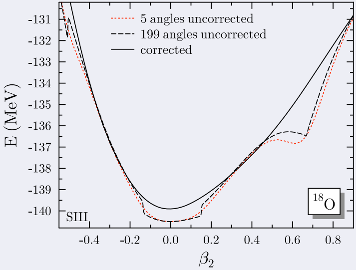
  3. Using SWT to compute $\langle\Phi_q|H|\Phi_{q'}\rangle/\langle\Phi_q|\Phi_{q'}\rangle$
  4. Extending to general EDF disconnected from genuine operator H
- GWT-inspired $\mathcal{E}[\Phi_q;\Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q\,*}]$ unsafe in EDF context
  1. Provides dangerous weights to terms that are zero with SWT
  2. Such terms cancel for WF method but not for more general EDF
  3. Originates from self interaction and self pairing in the EDF kernel

[D. Lacroix, T. D., M. Bender, PRC 79 (2009) 044318]

Regularization method

Regularized PNR calculations

- $\mathcal{E}_{REG}[\Phi_0;\Phi_\varphi] \equiv \mathcal{E}[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\,*}] - \mathcal{E}_C[\langle\Phi_0|;|\Phi_\varphi\rangle]$
  1. Analytical over $\mathbb{C}^*$
  2. $\mathcal{E}^{MR}_N$ is free from divergencies/steps and zero for $N \leq 0$



- The correction
  1. is crucial at critical points but also *away* from them
  2. depends on the quadrupole deformation ρ_{20}
  3. is on the MeV scale = mass accuracy/spectroscopic scale

[M. Bender, T. D., D. Lacroix, PRC 79 (2009) 044319]

Outline

Summary

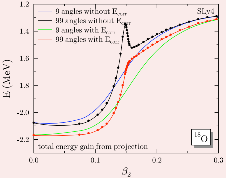
MR-EDF method

1. Efficient to tackle long-range correlations and access spectroscopy
2. Difficulties must be taken seriously

[J. Dobaczewski, W. Nazarewicz, P. G. Reinhard, M. V. Stoitsov, PRC76 (2007) 054315]

Regularization method

1. Valid for all MR modes; i.e. fluctuations of any $|q|$ and/or φ
2. Successful application to particle number restoration
3. Limited to EDF kernels of the form $\mathcal{E}[\rho^n, (\kappa^* \kappa)^m]$
4. Specific case of $\mathcal{E}[\rho^\gamma]$ with γ non integer



[T. D., M. Bender, K. Bennaceur, D. Lacroix, T. Lesinski, PRC 79 (2009) 044320]

Perspectives

To be done in the near future

1. Build correctable EDF of the form $\mathcal{E}[\rho^n, (\kappa^* \kappa)^m]$

   [J. Sadoudi, T. D., M. Bender, K. Bennaceur, in progress]

2. Build SI- and SP-free EDF

3. Perform regularized MR calculations for AMR and $\Delta\rho_{20}$ mixing

   [M. Bender, T.D., D. Lacroix, in progress]

4. Work out new constraints on $\mathcal{E}[\Phi_0; \Phi_\Omega]$ for various symmetry groups

$$\mathcal{E}[\Phi_0; \Phi_\Omega] \langle \Phi_0 | \Phi_\Omega \rangle = \sum_{\lambda ab} c^*_{\lambda a} \, c_{\lambda b} \, \mathcal{E}_\lambda \, S^\lambda_{ab}(\Omega)$$

   [T. D., J. Sadoudi, J. Phys. G: Nucl. Part. Phys, in press]

5. Need a constructive framework for MR-EDF method

Outline

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