

Consistent prescriptions for density dependent interactions in beyond mean field calculations

L.M. Robledo

Universidad Autónoma de Madrid
Spain

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Phenomenological effective (**density dependent**) interactions like Skyrme or Gogny and the **mean field approximation** represent a successful approach to low energy nuclear structure studies.

New accelerators, detectors and experimental setups allow more precise measurements of nuclear properties and access to new regions of the nuclear chart

The **mean field approximation** is, in many cases, too limited to deal properly with the nuclear many body problem and it is necessary to go beyond mean field to provide a more accurate description of low energy nuclear structure all over the Nuclear Chart.

A typical example is the ground state of ^{32}Mg

- Experimentally, its quadrupole deformed nature has been quite unambiguously established
- With all the reasonable parameterizations of the Skyrme or Gogny interactions the ground state is spherical at the mean field level
- Only after considering angular momentum projection and quadrupole configuration mixing the calculations give a quadrupole deformed ground state

Improving the mean field approach

- Vibrations of small amplitude (RPA)
- Shape coexistence and large amplitude motion (GCM)
- Restoration of broken symmetries (Projection)

In the last two cases one has to deal with linear combinations of mean field wave functions (HF or HFB) $|\Phi(q)\rangle$

$$|\Psi\rangle = \int dq f(q) |\Phi(q)\rangle$$

Hamiltonian and norm overlaps

$$\mathcal{H}(q, q') = \langle \Phi(q) | \hat{H} | \Phi(q') \rangle \quad \mathcal{N}(q, q') = \langle \Phi(q) | \Phi(q') \rangle$$

Density dependent interactions

$$V_{DD}(\rho) = t_3 \delta(\vec{r}_1 - \vec{r}_2) \rho^\alpha \left(\frac{1}{2} (\vec{r}_1 + \vec{r}_2) \right)$$

- Inspired by the results of Brueckner type calculations
- It is extremely hard (if not impossible) to deduced them from first principles
- They produce a **strongly repulsive interaction energy**
- State dependent interaction.
To compute $\langle \Phi | \hat{H}_{DD} | \Phi \rangle$ we use $\hat{H}_{DD} = f[\rho]$ with $\rho = \langle \Phi | \hat{\rho} | \Phi \rangle$

how to define the DD interaction for hamiltonian overlaps ?

Prescriptions for the density dependent interaction

A prescription is required for the calculation of $\langle \Phi(q) | \hat{H} | \Phi(q') \rangle$ in order to compute **energies**

As some of the prescriptions lead to complex and/or symmetry breaking density dependent terms we have to make sure they yield

- 1 Real energies
- 2 Energies that are invariant under symmetry transformations (scalar)

we also want to have a framework **consistent with the underlying mean field approximation**

- 1 Reduce to the mean field DD term when $|\Phi(q)\rangle = |\Phi(q')\rangle$
- 2 Produce consistent results for "mean field like" quantities like
 - Chemical potentials
 - RPA equation

Possible prescriptions used and/or proposed in the literature are

- **Mixed** density $\rho_{q,q'} = \langle \Phi(q) | \hat{\rho} | \Phi(q') \rangle / \langle \Phi(q) | \Phi(q') \rangle$
- **Average** density: $V_{DD} \propto \frac{1}{2}(\rho_{q,q}^{\alpha} + \rho_{q',q'}^{\alpha})$
- **Correlated** density

$$\int dq dq' f^*(q) f(q') \langle \Phi(q) | \hat{\rho} | \Phi(q') \rangle / \int dq dq' f^*(q) f(q') \langle \Phi(q) | \Phi(q') \rangle$$

This includes symmetry preserving densities like the projected density to $J=0$, etc

In the following it will be shown that only the **Mixed** density satisfies all the consistency requirements in spite of being complex and breaking some of the fundamental symmetries (rotational invariance, etc)

Mixed density $\rho_{q,q'} = \langle \Phi(q) | \hat{\rho} | \Phi(q') \rangle / \langle \Phi(q) | \Phi(q') \rangle$

- Inspired by the extended Wick theorem.
 $\frac{\langle \Phi(q) | \hat{H} | \Phi(q') \rangle}{\langle \Phi(q) | \Phi(q') \rangle}$ is written in terms of the the overlap density and overlap pairing tensors $\rho_{q,q' kl} = \frac{\langle \Phi(q) | c_l^+ c_k | \Phi(q') \rangle}{\langle \Phi(q) | \Phi(q') \rangle}$, etc is the same way as the expression of the energy is written in terms of the standard density and pairing tensor
- The right one when the density dependence comes from a three body force (Skyrme) in spin saturated systems.
- Right limit when $q = q'$

The mixed density is in general a complex quantity ! and might break symmetries !

Average density $V_{DD} \propto \frac{1}{2}(\rho_{q,q}^{\alpha} + \rho_{q',q'}^{\alpha})$

- Suggested by a LDA of a generalized Bruckner expansion for hamiltonian overlaps (Duguet, PRC 67 054308, 2003)
- Right limit when $q = q'$
- The DD term is real but might break symmetries

Correlated density

$$\int dq dq' f^*(q) f(q') \langle \Phi(q) | \hat{\rho} | \Phi(q') \rangle / \int dq dq' f^*(q) f(q') \langle \Phi(q) | \Phi(q') \rangle$$

- Symmetry invariant density dependent terms when f is choosen in the appropriate way
- The DD term is real
- Does not reduce to the standard when $q = q'$ and therefore, it should be also used at the mean field level.

Real energies

As both the average and correlated densities are real and positive definite they trivially satisfy this condition

The mixed density is in general a complex quantity but

$$E = \int dq dq' f^*(q) f(q') \langle q | \hat{H} | q' \rangle \quad E^* = \int dq dq' f(q) f^*(q') \langle q | \hat{H} | q' \rangle^*$$

and

$$\langle q | \hat{H} | q' \rangle^* = \langle q' | \hat{H}^\dagger | q \rangle \quad \hat{H}^\dagger[\rho_{q,q'}] = \hat{H}[\rho_{q',q}]$$

Therefore

$$E = E^*$$

R. R-G, J.L.E, L.M.R.; Nuclear Physics A709 (2002) 201

Symmetry requirements

Angular momentum projection will be discussed. For rotational invariant (scalar) hamiltonians we have

- $\langle \Psi_{IM} | \hat{H} | \Psi_{I'M'} \rangle = \delta_{II'} \delta_{MM'} \langle \Psi_{IM} | \hat{H} | \Psi_{IM} \rangle$
- $\langle \Psi_{IM} | \hat{H} | \Psi_{IM} \rangle = \langle \Psi_I | \hat{H} | \Psi_I \rangle$

where $|\Psi_{IM}\rangle = \frac{2I+1}{8\pi^2} \sum_K g_K \int d\Omega \mathcal{D}_{MK}^{I*}(\Omega) \hat{R}(\Omega) |\Phi\rangle = \sum_K \hat{P}_{MK}^I |\Phi\rangle$

which is a consequence of $[\hat{R}(\Omega), \hat{H}] = 0$ as it implies

$$\langle \Phi | \hat{R}^\dagger(\Omega') H \hat{R}(\Omega) | \Phi \rangle = \langle \Phi | H \hat{R}(\Omega' - \Omega) | \Phi \rangle$$

and therefore

$$\langle \Phi | P_{MK}^I{}^\dagger H P_{M'K'}^{I'} | \Phi \rangle = \langle \Phi | H P_{MK}^I{}^\dagger P_{M'K'}^{I'} | \Phi \rangle = \delta_{II'} \delta_{MM'} \langle \Phi | H P_{KK'}^{I'} | \Phi \rangle$$

Symmetry requirements

The previous requirement is fulfilled by the correlated density if we consider it to be the $J=0$ angular momentum projected one.

For the average and mixed density it is required that

$$\langle \Phi | \hat{R}^\dagger(\Omega') H_{DD}[\Omega', \Omega] \hat{R}(\Omega) | \Phi \rangle = \langle \Phi | H_{DD}[0, \Omega' - \Omega] \hat{R}(\Omega' - \Omega) | \Phi \rangle$$

but we have in general

$$\hat{R}^\dagger(\Omega') \rho(\vec{R}, \Omega', \Omega) \hat{R}(\Omega) = \rho(\vec{R}, 0, \Omega' - \Omega) \hat{R}(\Omega' - \Omega)$$

with

$$\rho(\vec{R}, \Omega', \Omega) = \frac{\langle \Phi | \hat{R}^\dagger(\Omega') \hat{\rho}(\vec{R}) \hat{R}(\Omega) | \Phi \rangle}{\langle \Phi | \hat{R}^\dagger(\Omega') \hat{R}(\Omega) | \Phi \rangle}$$

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Mean field chemical potential

- 1 At the mean field level and when particle number symmetry is broken (HFB) the routhian $\langle \hat{H} - \lambda \hat{N} \rangle$ is minimized with the constraint $\langle \hat{N} \rangle = N$.
- 2 The chemical potential λ is determined by the condition of having the gradient of the Routhian H' perpendicular to the gradient of the constraint

$$\lambda = \frac{\langle \hat{H} \Delta \hat{N} \rangle}{\langle \Delta \hat{N}^2 \rangle}$$

- 3 This procedure can be justified by starting from the particle number projected energy evaluated in an approximate way (the Kamlah expansion)

Mean field chemical potential

$$E^N = \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle} = \frac{\int d\varphi h(\varphi) e^{-iN\varphi}}{\int d\varphi n(\varphi) e^{-iN\varphi}} \quad \frac{n(\varphi)}{h(\varphi)} = \langle \Phi | \frac{1}{H} e^{i\hat{N}\varphi} | \Phi \rangle$$

Kamlah expansion

$$h(\varphi) = \sum_{m=0}^M h_m \hat{I}^m n(\varphi) \text{ with } \hat{I} = -i\partial_\varphi - \langle N \rangle.$$

For $M=1$ we have $E_{M=1}^N = \langle \Phi | (H - h_1(\hat{N} - N)) | \Phi \rangle$ with

$$h_1 = \frac{\hat{I} h(\varphi)|_{\varphi=0}}{\langle \Delta \hat{N}^2 \rangle} = \frac{\langle \hat{H} \Delta \hat{N} \rangle}{\langle \Delta \hat{N}^2 \rangle}$$

The minimum of $E_{M=1}^N$ with the constraint $\langle \Phi | \hat{N} | \Phi \rangle = N$ is equivalent to minimizing $\langle \Phi | (H - h_1 \hat{N}) | \Phi \rangle$

Mean field chemical potential

- 1 For density dependent forces the chemical potential is computed in the same way but we have an extra **rearrangement term**

$$\langle (\hat{H} + \partial \hat{f}) \Delta \hat{N} \rangle - \lambda \langle \Delta \hat{N}^2 \rangle = 0 \quad \partial \hat{f} = \sum_{ij} \langle \frac{\delta H}{\delta \rho} \varphi_i^* \varphi_j \rangle c_i^\dagger c_j$$

- 2 To get $h_1 = \lambda$ for density dependent forces we must have

$$h_1 = \frac{\hat{I} h(\varphi)|_{\varphi=0}}{\langle \Delta \hat{N}^2 \rangle} = \frac{\langle (\hat{H} + \partial \hat{f}) \Delta \hat{N} \rangle}{\langle \Delta \hat{N}^2 \rangle}$$

implying that the DD term **MUST** depend upon φ .

The only prescription satisfying this requirement is the **mixed** density.

RPA

The RPA equation can be derived as a special limit of the Time Dependent Mean Field (HF or HFB) equations.

For Density Dependent forces (Blaizot&Gogny) the interaction matrix elements entering the RPA equation are given by the second derivative

$$\frac{\delta^2 E}{\delta \rho_{ij} \delta \rho_{kl}}$$

Rearrangement terms ! that is, derivatives of the density dependent interaction have to be considered in the RPA matrix elements

The RPA can also be derived from the GCM (Jancovici&Schiff, Brink &Weiguny)

- $|\mathbf{Z}\rangle = \exp(\sum_{\mu\nu} Z_{\mu\nu} \alpha_{\mu}^+ \alpha_{\nu}^+) |\psi_0\rangle$
- Expand $\langle \mathbf{Z}' | \hat{H} | \mathbf{Z} \rangle = \mathcal{H}(\mathbf{Z}'^*, \mathbf{Z})$ up to second order
- Assume Gaussian overlaps $\langle \mathbf{Z}' | \mathbf{Z} \rangle \propto \exp(-\mathbf{Z}'^* \mathbf{Z})$
- Introduce the above in the Hill-Wheeler equation
- After some manipulations the RPA equation is obtained

and the only way to get the same rearrangement terms as in the standard derivation of the RPA is to have a density dependent term depending upon $\mathbf{Z}'^*$ and $\mathbf{Z}$.

- **Mixed** density is OK
- **average** density is not OK as it depends also on $\mathbf{Z}'$ and $\mathbf{Z}^*$

The correlated density again

- 1 Very appealing in doing projection as it preserves the symmetries of the system as will do the DD interaction and therefore the hamiltonian.
- 2 Let us consider, for simplicity, parity projection. The intrinsic wave functions have an octupole moment Q_3 different from zero. The projector to good parity p is given by

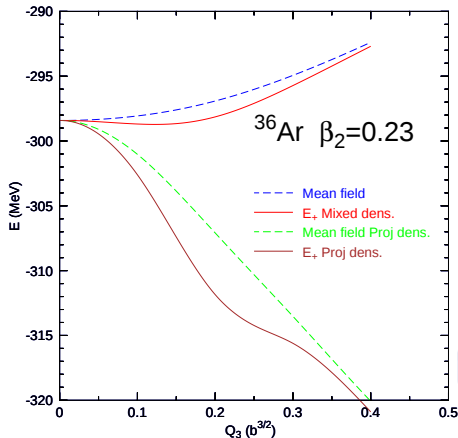
$$\hat{P}_p = 1 + p\Pi$$

- 3 The correlated density to be used is the one projected to **positive** parity

$$\rho_{Proj} = \frac{\langle \Psi | (1 + \Pi) \hat{\rho} (1 + \Pi) | \Psi \rangle}{\langle \Psi | (1 + \Pi) (1 + \Pi) | \Psi \rangle}$$

Such that $\rho_{Proj}(-\vec{r}) = \rho_{Proj}(\vec{r})$

An example



- 1 Standard

$$E_{DD} \propto \int d^3\vec{r} \rho^\tau(\vec{r}) \rho^{\tau'}(\vec{r}) \rho^\alpha(\vec{r})$$
- 2 ρ_{Proj} not the same shape as ρ

$$\rho_{Proj}(\vec{r}) \approx \rho(\vec{r}) + \rho(-\vec{r})$$
- 3 Integrand decreases
- 4 $t_3 \approx 1400$ MeV

Meaningless prescription!

Conclusions

- Density dependent interactions successfully describe many nuclear properties in the framework of the mean field
- Beyond-mean-field methods are becoming very important for the correct description of nuclear structure
- Density dependent interactions are not defined for hamiltonian overlaps which are needed for the beyond mean field methods
- Prescriptions for the density dependence must satisfy consistency requirements (real energies, etc)
- The mixed density satisfies all of them in spite of being a complex and symmetry breaking quantity
- The projected density prescription is meaningless