To what extent does the self-consistent mean-field exist?

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Introduction

HF mean-field theory has been applied successfully for various quantum many-fermion systems.

Various averaged quantities, a concept of mean-field has physical reality only when near stationary, locally homogeneous.

Mean-field with various correlations of the system as much as possible.

To what extent the concept of mean-field and average quantities have a sense? How and why it breaks down near level repulsion?

Level repulsion is a universal phenomenon, appearing in various fields of physics, like molecular, atomic, biological systems, quantum dot and atomic nucleus.
In the development of nuclear physics:

Many discussions on an applicability of the cranked mean-field near level repulsion

\[ \hat{H}' = \hat{H} - \omega \hat{j}_x \]

spurious interaction

large $I$ fluctuation

in deformation constraint mean-field theory: Non-spurious interaction

A competition between mean-field and two-body residual interaction

What actually happens in level repulsion in CHF theory

whether a concept of self-consistent mean-field is realized or not???
**Gogny-CHFB**

**CHF equation:**

\[ \delta \left( \langle \hat{H} \rangle + \frac{1}{2} w (\langle \hat{Q}_{20} \rangle - \mu)^2 + \frac{1}{2} \alpha_x \langle \hat{x} \rangle^2 \right) = 0, \]

with constraints

\[ \langle \Psi(q) | \hat{Q}_{20} | \Psi(q) \rangle = q, \]
\[ \langle \Psi(q) | \hat{x} | \Psi(q) \rangle = 0, \]

**Two-body interaction:** Gogny D1S, Coulomb, Center of mass motion

**Symmetries:**

\[ \hat{P} e^{-i \pi \hat{J}_z} \text{ (z-simplex)} \text{ and } \hat{P} e^{-i \pi \hat{J}_y} \hat{T} \text{ (} \hat{S}_y^T \text{)} \]

**Basis:** three dimensional harmonic oscillator
Methods to solve CHF(B) equation:

(a) Conventional adiabatic method:
the most energetically favorable CHF(B) state

(b) Configuration-dictated method:

\[
\lim_{\Delta q \to 0} \langle \varphi_i(q) | \varphi_j(q + \Delta q) \rangle = \delta_{i,j}, \quad i, j = 1, \ldots, N,
\]

In our calculation, the condition is taken as

\[
| \langle \varphi_i(q) | \varphi_i(q + \Delta q) \rangle |^2 > 0.9, \quad i = 1, \ldots, N.
\]

Excited states and continuously-connected CHF(B) lines

Fragility of mean-field

(a) difficulty of non-convergence near level repulsion in CHF theory

FIG. 1: CHF calculation for $^{66}$Se: (a) the calculated quadrupole moment as a function of input quadrupole moment parameter $\mu$; (b) binding energy as a function of quadrupole moment $q$. 
Nonlinear CHF equation

\[ [h, \rho] = 0 \]

In numerical basis:

\[ \rho_{\alpha\beta}^{(n)}(q) \equiv \sum_i \varphi_{\alpha i}^{(n-1)}(q) \varphi_{\beta i}^{(n-1)*}(q), \]

\[ \Gamma_{\alpha\beta}^{(n)}(q) \equiv \sum_{\gamma\delta} \bar{u}_{\alpha\gamma\beta\delta} \rho_{\delta\gamma}^{(n)}(q). \]

\[ h_{\alpha\beta}^{(n)}(q) \equiv t_{\alpha\beta} + \Gamma_{\alpha\beta}^{(n)}(q) - \chi^{(n)}(q) Q_{\alpha\beta}. \]

in the s.p. basis where \( h \) is diagonal

\[ \rho_{kk}^{(n)}(q) \equiv \sum_{\alpha\beta} \varphi_{\alpha k}^{(n)*}(q) \rho_{\alpha\beta}^{(n)}(q) \varphi_{\beta k}^{(n)}(q), \]

\[ \begin{align*}
\text{Fig. 2: Diagonal components of (a) proton and (b) neutron density as a function of iterations for a given non-convergent state } \mu = 150 \text{ fm}^2. \text{ The single-particle basis where } h \text{ is diagonal is used. Occ. and Unocc. stand for occupied and unoccupied orbits, respectively. } (\pi, \alpha) \text{ denotes the parity and signature, and its subscripts } A \text{ and } A+1 \text{ represent the orbits responsible for the non-convergent difficulty.}
\end{align*} \]
FIG. 3: Neutron s.p. energies near Fermi surface.
(b) microscopic dynamics of non-convergence and staggering properties

There exists CHF state at $q = q_0$, it will be explored whether or not one gets a convergent CHF state at $q = q_0 - \Delta q$?

To study dynamical change of s.p. wave function, a fixed basis is used in a $q_0$-representation of using s.p. states $\{\epsilon_k(q_0), \varphi_k(q_0)\}$ at

$$h_{kl}^{(n)}(q_0 - \Delta q) = \sum_{\alpha \beta} \varphi^*_{\alpha k}(q_0) h_{\alpha \beta}^{(n)}(q_0 - \Delta q) \varphi_{\beta l}(q_0)$$
For the \((A-1)\) number of hole-state, making an approximate expression

\[
\sum_{i=1}^{A-1} \varphi_{\alpha i}(q_0) \varphi_{\beta i}^*(q_0) \approx \sum_{i=1}^{A-1} \varphi^{(n)}_{\alpha i}(q_0 - \Delta q) \varphi^{(n)*}_{\beta i}(q_0 - \Delta q),
\]

Independent of \(\Delta \mu\) and \(n\)

The interacting \(A\)th and \((A+1)\)th states are expressed by unitary transformation

\[
\begin{pmatrix}
\varphi^{(n)}_A(q_0 - \Delta q) \\
\varphi^{(n)}_{A+1}(q_0 - \Delta q)
\end{pmatrix}
= U^{(n)}
\begin{pmatrix}
\varphi_A(q_0) \\
\varphi_{A+1}(q_0)
\end{pmatrix},
\quad
U^{(n)} = \begin{pmatrix}
 a^{(n)} & b^{(n)} \\
d^{(n)} & c^{(n)}
\end{pmatrix}.
\]

Non-convergent dynamics in terms of truncated Hamiltonian

\[
\begin{pmatrix}
 h^{(n)}_{A,A}(q_0 - \Delta q) & h^{(n)}_{A,A+1}(q_0 - \Delta q) \\
 h^{(n)}_{A+1,A}(q_0 - \Delta q) & h^{(n)}_{A+1,A+1}(q_0 - \Delta q)
\end{pmatrix}.
\]
The relations of off-diagonal Hamiltonian between \((n+1)\)th and \(n\)th iterations

\[
\begin{align*}
    h^{(n+1)}_{A, A+1} &= h^{(n)}_{A, A+1} + \left\{ a^{(n)} b^{(n)} - a^{(n-1)} b^{(n-1)} \right\} \left\{ \tilde{v}_{A+1 A A A+1} + 2wQ^2_{A, A+1} \right\} \\
    &+ w\left\{ b^{(n)} - b^{(n-1)} \right\} Q_{A, A+1}(Q_{A+1, A+1} - Q_{A, A}),
\end{align*}
\]

between \((n+2)\)th and \(n\)th iterations

\[
\begin{align*}
    h^{(n+2)}_{A, A+1} &= h^{(n)}_{A, A+1} + \left\{ a^{(n+1)} b^{(n+1)} - a^{(n-1)} b^{(n-1)} \right\} \left\{ \tilde{v}_{A+1 A A A+1} + 2wQ^2_{A, A+1} \right\} \\
    &+ w\left\{ b^{(n+1)} - b^{(n-1)} \right\} Q_{A, A+1}(Q_{A+1, A+1} - Q_{A, A}).
\end{align*}
\]

satisfied for both convergent and non-convergent cases

\[
\text{if } \text{sign}(a^{(n)} b^{(n)}) \begin{cases} \text{same convergence} & \text{change non-convergence} \\ \end{cases} \Rightarrow \tilde{V}_{A+1 A A A+1}
\]

For detailed analytic derivation, please see nucl-th/0407031, nucl-th/0408050.

And anti-symmetric two-body interaction

\[
\tilde{v}_{k_1 k_2 k_3 k_4} \equiv \sum_{\alpha/\beta/\gamma/\delta} \varphi^*_{\alpha k_1}(q_0) \varphi^*_{\gamma k_2}(q_0) \tilde{v}_{\alpha\gamma\beta\delta} \varphi_{\beta k_3}(q_0) \varphi_{\delta k_4}(q_0).
\]
Matrix diagonalization gives:

\[
\text{sign}(a^{(n)} b^{(n)}) = \text{sign}\left(h_{A,A+1}^{(n)} / (h_{A,A}^{(n)} - h_{A+1,A+1}^{(n)})\right)
\]

Physically, two mean-fields, one characterized by \(\varphi_A(q_0)\) with different sign and the other by \(\varphi_{A+1}(q_0)\) with same sign interact too strongly by two body residual interaction to be approximated by a single mean-field.

FIG. 5: For the given non-convergent state \(\mu = 150 \text{ fm}^2\) (a) the off-diagonal Hamiltonian and difference of diagonal components as a function of iterations; (b) the relative phase of wave function for the specific orbit \((-,-)_A\). CHF eigenstate at the critical point is taken as the single-particle basis in numerically representing \(h\) and \(ab\).
Matrix diagonalization gives:

\[
\text{sign} (a^{(n)} b^{(n)}) = \text{sign} \left( \frac{h_{A,A+1}^{(n)}}{h_{A,A}^{(n)} - h_{A+1,A+1}^{(n)}} \right)
\]

In convergent situation, same sign among

\[
a^{(n+1)} b^{(n+1)} \quad a^{(n)} b^{(n)} \quad a^{(n-1)} b^{(n-1)}
\]

FIG. 6: Same as Fig. 5, except for the given convergent state \(\mu = 180 \text{ fm}^2\).

Two-body residual interaction is successfully incorporated into mean-field
analytic condition on applicability of mean-field theory

There exists a self-consistent mean-field, when there holds a condition

$$\frac{h_{A,A+1}^{(n+1)}}{h_{A,A+1}^{(n)}} \geq 0,$$

Is decided by

$$\left\{ \frac{h_{A,A+1}^{(2)}}{h_{A,A+1}^{(1)}} \right\} \geq 0.$$

$$\text{sign} \left\{ \frac{h_{A,A+1}^{(2)}}{h_{A,A+1}^{(1)}} \right\}$$

$$= \text{sign}\{\epsilon_{A+1}(q_0) - \epsilon_{A}(q_0) - (\bar{v}_{A+1A1}A + 2wQ_{A,A+1}^2) - w\Delta\mu (Q_{A,A} - Q_{A+1,A+1}) - O(b)\},$$

where $O(b)$ contains a small mixing parameter $b^{(1)}$

$$O(b) = -2b^{(1)}^2(\bar{v}_{A+1A1}A + 2wQ_{A,A+1}^2) + \frac{wb^{(1)}}{a^{(1)}} \left( 1 - 2b^{(1)}^2 \right) Q_{A,A+1}(Q_{A+1,A+1} - Q_{A,A}).$$
The condition to apply CHF mean-field successfully

\[ \epsilon_{A+1}(q_0) - \epsilon_A(q_0) \geq \bar{v}_{A+1A}A_{A+1} + 2wQ_{A,A+1}^2 + w\Delta \mu (Q_{A,A} - Q_{A+1,A+1}) + O(b), \]

Physically, two-body correlation between nucleons can be successfully incorporated into the mean-field as much as possible when.....

the well-known stability matrix of mean-field theory:

\[ \delta = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \]

\[ A = (\epsilon_m - \epsilon_i) + \bar{V}_{mjin} \quad B = \bar{V}_{mnij} \]

\[ \epsilon_{A+1} - \epsilon_A \quad \text{quant. fluc.} \]

\[ 2wQ_{A,A+1}^2 + w\Delta \mu (Q_{A,A} - Q_{A+1,A+1}) \]

FIG. 7: (a) The energy difference between two specific orbits and quantum fluctuations as a function of quadrupole moment \( q \); (b) the s.p. energy difference, two-body residual interaction and the sum of deformation fluctuation and quadrupole deformation as a function of quadrupole moment \( q \).
The condition that CHF mean-field breaks down

$$\epsilon_{A+1}(q_0) - \epsilon_A(q_0) < \bar{v}_{A+1AAA+1} + 2wQ_{A,A+1}^2 + w\Delta\mu(Q_{A,A} - Q_{A+1,A+1}) + O(b),$$

**FIG. 6:** The ratio of off-diagonal components between the first and second iterations for each given $\mu$. 
Conclusion

- Non-convergent difficulty near level repulsion
- Analytic condition to indicate the breakdown of CHF

\[ \epsilon_{A+1}(q_0) - \epsilon_{A}(q_0) < \bar{\nu}_{A+1AAA+1} + 2wQ_{A,A+1}^2 + w\Delta \mu(Q_{A,A} - Q_{A+1,A+1}) + O(b), \]

- Analytic condition works well for realistic situation