Open problems in particle-vibration coupling (PVC) calculations

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Outline

• Global research line: go beyond HF-RPA in a rigorous many-body scheme.

• Particle-vibration coupling (PVC) in a general framework. **Problem #1**: density-dependent forces or density functionals.

• Present status of PVC calculations – focused on the width and line shape of giant resonance and on particle-phonon multiplets. **Problem #2**: why are these results much better than those on s.p. states?

• **Problem #3**: regularization of effective forces for beyond mean-field calculations: infinite matter and finite nuclei.
Bottom line

We want to do PVC calculations because this is the most effective way, if not the only one, to explain *fragmentation and widths* of single-particle and giant resonances in a consistent fashion.
Co-workers

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- H. Sagawa (University of Aizu and RIKEN, Japan)
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Many-body theory vs. EDF

First motivation of our study: if the practical realization of the EDF has shortcomings, other kinds of calculations are useful.

\[ E = E \left[ \rho_q \text{ plus gradients, spin densities, ...} \right] \]

No exact prescription on how to build it!

Second motivation of our study: Some phenomena are, by definition, outside the EDF framework: fragmentation of the s.p. strength, width of collective states …
Beyond mean field (HF plus RPA)

• In a many-body language HF (or RPA) turn out to be the simplest approximations to describe single-particle (or collective) states: they are mean-field approximations.

• In nuclear physics these approximations can be highly successful as a large class of many-body correlations are included when the effective interactions are fitted. So, they are believed to realize DFT or TDDFT in atomic nuclei.

• Still, there are – or may be – dynamical processes that one cannot describe without explicit time-dependence.

\[ \rho(r, r') \equiv G(r, t, r', t' = t^+) \quad U(r, r') \equiv \Sigma(r, t, r', t' = t^+) \]

In the following: \( 1 \equiv (\vec{r}, t), \quad 2 \equiv (\vec{r}', t') \ldots \)
Our many-body approach

\[ H = H_0 + V_{\text{eff}} \]

\[ \sum_i \varepsilon_i a_i^\dagger a_i + \frac{\delta^2 H}{\delta \rho \delta \rho} \]

Equations for \( G, M, W, \Pi, \Gamma \) can be derived

- The set of equations for these quantities has been derived in the famous paper(s) by L. Hedin for the Coulomb force.
- PVC is a well-defined approximation scheme (first iteration of the Hedin’s equations).
- We have extended these equations in the case of DD interactions (?).
- The validity of this scheme when a functional is given can be discussed.

L. Schiacchitano, M.Sc. Thesis, University of Milano (unpublished);
M. Baldo et al.
Our Skyrme HF-RPA implementation

The continuum is discretized. The basis must be large due to the zero-range character of the force. Parameters: $R, E_C$.

Full self-consistency: the EWSR should be equal to the double-commutator value: well fulfilled!

$$m_1(\hat{O}) = \sum_{\nu} E_\nu |\langle \nu | \hat{O} | \bar{0} \rangle|^2 = \frac{1}{2} \langle 0 | [\hat{O}, [H, \hat{O}]] | 0 \rangle$$

$^{208}$Pb - SGII

Percentages $m_1(\text{RPA})/m_1(\text{DC})$ [%]
Consistent treatment of
- all standard Skyrme terms
- direct Coulomb interaction
- exchange Coulomb in Slater approximation
- one-body center-of-mass correction

\[ m' = m \frac{A}{A - 1} \]

is essential for such accurate fulfillment of EWSRs.

G. Colò, L. Cao, N. Van Giai, L. Capelli
Particle-vibration coupling for s.p. states

\[ M = iG^0 W \]

This PVC diagram can be extracted from second-order perturbation theory.

Phenomenologically, it can be introduced by simply considering the particles and the vibrations as independent degrees of freedom (Copenhagen, Dubna...).

However, we now perform calculations without any free parameter, or any experimental input, since we use the Skyrme force consistently (RMF: cf. E. Litvinova, P. Ring and A. Afanasjev).
Results for $^{208}\text{Pb}$

R.m.s. deviation experimental vs. theoretical energies (T44)

- HF: 1.42 [MeV]
- PVC (central): 1.00
- PVC (including spin-orbit): 0.91
- PVC (including tensor): 0.87

Effective mass $m^*/m$

- HF: 0.84
- PVC (central): 0.97
- PVC (including spin-orbit): 1.00
- PVC (including tensor): 1.04

PVC with proper treatment of continuum

The Dyson equation is written in coordinate space with proper continuum HF wavefunctions, and phonons from continuum-RPA. Adequate for weakly-bound systems.

\[ G = G^0 + G^0 M G \]
\[ [\omega - H_0] G(\vec{r}, \vec{r}'; \omega) = \delta(\vec{r} - \vec{r}') + \int d^3 r' M(\vec{r}, \vec{r}'; \omega) G(\vec{r}, \vec{r}'; \omega) \]

Even in the case of stable nuclei, we may need this to analyze state in (or close to) the continuum. **Y-axis:** spectral density. Red=exp. Blue=theory.

The RPA plus PVC (here the self-energy is $\Sigma$)

\[
\begin{pmatrix}
A + \Sigma(E) & B \\
-B & -A - \Sigma^*(-E)
\end{pmatrix}
\Sigma_{php'h'}(E) = \sum_{\alpha} \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E - E_\alpha + i\eta}
\]

The state $\alpha$ is 1p-1h plus one phonon.

The scheme is known to be effective to produce the spreading width of GRs.

Pauli principle ! (So far, only genuine collective states selected).

As in the case of s.p. states, fully self-consistent implementation.
The quadrupole response in $^{208}$Pb

- **Isoscalar** (*PRC* 85, 014305 (2012))

  - $E_{ISGQR} = 11.3 \text{ MeV} \ (10.9 \pm 0.3 \text{ MeV})$
  - $\Gamma_{ISGQR} \approx 2.3 \text{ MeV} \ (3.0 \pm 0.3 \text{ MeV})$

- **Isovector** (*PRC* 87, 034301 (2013))

  - $E_{IVGQR} = 22.0 \text{ MeV} \ (20.2 \pm 0.5 \text{ MeV})$
  - $\Gamma_{IVGQR} \approx 4 \text{ MeV} \ (5.5 \pm 0.5 \text{ MeV})$
  - Exp. *PRL* 68, 3507 (1992)
The Giant Dipole Resonance in $^{120}$Sn

\[ \frac{N}{2A} \sum_{i=1}^{Z} r_i Y_{1M}(\Omega_i) - \frac{Z}{2A} \sum_{i=1}^{N} r_i Y_{1M}(\Omega_i) \]

Figure 5. Photoabsorption cross section for $^{120}$Sn, calculated with the QRPA (vertical bars) and QRPA-PC (solid curve). The theoretical results are shown in comparison with experimental values.

Application to Gamow-Teller Resonances

- The energy shift induced by PVC is very weakly interaction-dependent.
- The PVC calculations reproduce the lineshape of the GT response very well.

Y. Niu et al., PRC (submitted).
Application to particle-phonon multiplets

There are well-known multiplets, made up in odd nuclei from particle plus phonon states.

They complement the understanding of particle-vibration coupling from single-particle states.

Example: $^{49}$Ca ground state is $3/2^-$, and there are states coming from: $\left[p_{3/2} \otimes 3^-\right]_{J^\pi=3/2^+ \ldots 9/2^+}$

Exp: $^{64}$Ni + $^{48}$Ca @ 5.7 MeV/A

- Nuclei around $^{48}$Ca populated by transfer reactions
- Angular momentum alignment perpendicular to the reaction plane $\rightarrow$ gamma-spectroscopy allows determining the multiplicity (through angular distribution)
- $^{49}$Ca: a first case analyzed in detail!
Old (d,p) experiment.

Hypothesis: states built with a $f_{7/2}$ or $p_{3/2}$ neutron coupled with a $^{48}\text{Ca}$ phonon.


New experiment: confirmation of the PVC hypothesis by means of the electromagnetic transition probabilities.
We start from a basis made up with particles (or holes) around a core, and with vibrations of the same core (i.e., phonons).

\[
\begin{bmatrix}
\varepsilon_i \\
\langle i|V|k_1L_1\rangle/j_i \\
\langle i|V|k_1L_1\rangle/j_i & \varepsilon_{k_1} + \omega_{L_1} \\
\langle i|V|k_2L_2\rangle/j_i & 0 & \varepsilon_{k_2} + \omega_{L_2} \\
& 0 & 0 & \ldots
\end{bmatrix}
\]

Relationship with the SM formulation could be formulated.
Re-fit of the force and divergences

- Our results show that the Skyrme forces provide reasonable results even when employed beyond mean field.

- However, in principle one should re-fit the parameters when the framework in which the effective force is used is changed.

- A zero-range force produce divergences in diagrams that appear in new approximations beyond mean field.

- The problem is common to Gogny sets, and some of the RMF Lagrangians.
Zero-range forces and ultraviolet divergences

We start from the divergence of “prototype” diagrams, corresponding to the second-order corrections to the energy, when a zero-range force is employed.

\[ V(r_1, r_2) = g \delta(r_1 - r_2) \]

We consider, as a start, the case of uniform systems (momentum labels). We study \( E/A(\text{HF}) + \Delta E^{(2)}/A \).

Divergence evident from power counting (linear).

\[ \sim \int d_3q \frac{v^2(q)}{q^2} \]
Cutoff renormalization in the simplest case

We include a momentum cutoff $\Lambda$ among the parameters of the interaction, and we show that for every value of $\Lambda$, the remaining parameters can be determined in such a way that the total energy of the system remains the same.

Same philosophy as standard QED.

Formulas are general. Useful for atomic gases!

Numerical application is for nuclear matter.

$$V(r_1, r_2) = g \delta(r_1 - r_2)$$

A simplified Skyrme force is employed ($t_0, t_3$).

Our benchmark is the EOS obtained with the set SkP.

Beyond Mean-Field Theories with Zero-Range Effective Interactions: A Way to Handle the Ultraviolet Divergence

K. Moghrabi, M. Grasso, G. Colo, and N. Van Giai
• The divergence is studied in detail for different densities.

$$\Delta E = \frac{d \frac{\Omega^3}{(2\pi)^6}}{\int_{k_1, k_2 < k_F, |k_1 + q|, k_2 - q| > k_F} d^3k_1 d^3k_2 d^3q \frac{v^2}{\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1 + q} - \epsilon_{k_2 - q}}} = \chi(\rho) \times I(\rho, \infty).$$

$$I(\rho, \Lambda) = \frac{1}{105} (43 - 46 \ln 2) - \frac{18}{35} + \frac{\Lambda}{35 k_F} + \frac{11 \Lambda^3}{210 k_F^3} + \frac{\Lambda^5}{840 k_F^5} + \frac{16 \ln 2}{35} + \left( \frac{\Lambda^5}{60 k_F^5} - \frac{\Lambda^7}{1680 k_F^7} \right) \ln \left( \frac{\Lambda}{k_F} \right) + \left( \frac{1}{35} - \frac{\Lambda^2}{30 k_F^2} + \frac{\Lambda^4}{48 k_F^4} + \frac{\Lambda^5}{120 k_F^5} - \frac{\Lambda^7}{3360 k_F^7} \right) \ln \left( 2 + \frac{\Lambda}{k_F} \right).$$

• For every $\Lambda$ we build a new SkP$_\Lambda$ such that the EOS does not change.
• This work has now been extended to the case of the complete Skyrme force \((t_0, t_1, t_2, t_3)\), both for symmetric and asymmetric matter.

\[
\delta \equiv \frac{\rho_n - \rho_p}{\rho}
\]

• The important feature is that for every value of the cutoff \(\Lambda\), there is a unique fit for all values of the asymmetry! This paves the way to calculations for finite nuclei.

Renormalization in finite nuclei

- We cannot use the transferred momentum like in infinite matter.

\[ \langle k_1 k_2 | V | k_3 k_4 \rangle \]

\[ k_3, k_4 \in \text{particles} \]

\[ \frac{k_3 - k_4}{\sqrt{2}} \quad \frac{k_3 + k_4}{\sqrt{2}} \]

- Following the original spirit of T.H.R. Skyrme’s papers, we impose a cutoff on the relative momentum [cf. also \( V_{\text{low-k}} \) and PRC 87, 054303 (2013)].

\[ \lambda = \sqrt{2} \Lambda \]

- The dependence on the maximum energy of particles has also to be checked.

\[ \varepsilon_p^{\text{max}} \]

A second scale…
Only $t_0$, $t_3$ part of the force SkP.

The second order energy clearly diverges.

Our scope is:

- Take the parameters of the interaction that has been renormalized in nuclear matter;
- Use it for the finite nucleus:
  \[ \lambda = \sqrt{2} \Lambda \]
- Goal: check if we can reabsorb the divergence in the total energy $E + \Delta E$;
- We must check the dependence on the maximum energy of the particle as well.
Renormalized interaction ("Skyrme_{low-k}")

- Interaction (velocity independent terms) written in order to identify initial and final channels, in the center of mass and relative motion coordinates

\[
g(r) = t_0 + \frac{t_3}{6} \rho(r)^\alpha
\]

\[
V(r_1', r_2', r_1, r_2) = \frac{\sqrt{2}}{4} g\left(\frac{R}{\sqrt{2}}\right) \delta(r') \delta(r) \delta_3(R - R')
\]

\[
= \frac{\sqrt{2}}{4} g\left(\frac{R}{\sqrt{2}}\right) v(r', r) \delta_3(R - R'),
\]

where \( r^{(i)} = \frac{r_1^{(i)} - r_2^{(i)}}{\sqrt{2}} \) and \( R^{(i)} = \frac{r_1^{(i)} + r_2^{(i)}}{\sqrt{2}} \)

- We introduce two cutoffs \( \lambda \) and \( \lambda' \) on initial and final relative momenta

\[
v^{\lambda\lambda'}(r', r) = \frac{1}{\Omega} \int d^3 k d^3 k' e^{i k' \cdot r'} v(k', k) \theta(\lambda - k) \theta(\lambda' - k') e^{-i k \cdot r}
\]

\[
= \frac{1}{4\pi^2} \frac{\lambda^2 \lambda'^2}{r r'} j_1(r \lambda) j_1(r' \lambda')
\]

- The interaction acquires a finite range
Since we want to separate the center-of-mass and relative coordinate degrees of freedom, we work in harmonic oscillator basis.

We choose a cutoff $\lambda$ that corresponds to the cutoff $\Lambda$ in infinite matter.

We use the same interaction that has been already renormalized in infinite matter.

We solve HF and add the second-order contribution to the energy.

We are consistent but we use perturbation theory.
$$\Delta E \equiv \frac{1}{4} \sum_{pp',hh',J} \frac{|\langle hh'|J|V|(pp')J \rangle|^2}{\varepsilon_h + \varepsilon_{h'} - \varepsilon_p - \varepsilon_{p'}}$$

$$\langle (n_al_{j_a}a_{\tau_a}, n_b|b_{j_b} b_{\tau_b}) |J\rangle |V| (n_c|c_{j_c} c_{\tau_c}, n_d|d_{j_d}d_{\tau_d}) |J\rangle \rangle_I =$$

$$= N_I F_I \sum_{\Sigma L} i^{-l_a-l_b+l_c+l_d} L^2 \Sigma^2 \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d G_I \left\{ \begin{array}{ccc} l_a & l_b & L \\ \frac{1}{2} & \frac{1}{2} & \Sigma \\ j_a & j_b & J \end{array} \right\} \left\{ \begin{array}{ccc} l_c & l_d & L \\ \frac{1}{2} & \frac{1}{2} & \Sigma \\ j_c & j_d & J \end{array} \right\}$$

$$\frac{\chi^2 \lambda^2}{\pi^3} \sum_{\frac{n_iN_i}{n_fN_f}} M_L(N_fLn_f0; n_al_an_b|b) M_L(N_iLn_i0; n_c|c n_d|d) \int dRR^2 R_{N_fL}(\sqrt{2}\beta R)g(R)R_{N_iL}(\sqrt{2}\beta R)$$

$$\int dr rR_{n_{i0}}(\beta r)j_1(r\lambda) \int dr' r'R_{n_{f0}}(\beta r')j_1(r'\lambda').$$

- From $jj$ to LS coupling
- HO basis
- Transformation to proper coordinate system (Brody-Moshinsky coefficients)
In a region between $\lambda \approx 2$ and $3 \text{ fm}^{-1}$ the results for the TOTAL energy are quite stable. The result is also stable with respect to variations of the maximum energy of the particles $\varepsilon_p^{(\text{max})}$, provided this is not too small. This can be understood with semiclassical arguments.
Results (II)

For small values of the cutoff the system is not bound, or anyway far from its expected configuration. We cannot expect perturbation theory to work.

For those values of the cutoff the system is even “dilute”. But for higher values of the cutoff the starting point is quite reasonable!
Results (III)

• Stability with respect to the maximum particle energy: visible in the left panel.

• Large cutoff: numerical problems? Breakdown of perturbative approach?

• Full solution of Dyson equation, and evaluation of the total energy using Koltun sum rule, envisaged.
Conclusions

• We have at our disposal a formal many-body theory to go beyond mean-field, along the spirit of particle-vibration coupling.

• It is possible to avoid uncontrolled approximations and use consistently some microscopic Hamiltonian.

• As a rule, width of giant resonances is better reproduced than detailed spectra of s.p. states.

• There have been not much attempts, so far, to re-fit interactions that have been fitted at the mean-field level.

• As a first step in this direction we have proposed a route to re-absorb divergences that arise beyond mean-field when using zero-range forces.

• Promising results for a finite nucleus just obtained!