Microscopic theory of particle-vibration coupling

Gianluca Colò, Pier Francesco Bortignon
Dipartimento di Fisica, Università degli Studi di Milano and INFN, Sez. di Milano, via Celoria 16, 20133 Milano (Italy)
E-mail: colo@mi.infn.it

Hiroyuki Sagawa
Center for Mathematics and Physics, University of Aizu, Aizu-Wakamatsu, Fukushima 965-8560 (Japan)

Kassem Moghrabi, Marcella Grasso, Nguyen Van Giai
Institut de Physique Nucléaire, Université Paris-Sud, IN2P3-CNRS, 91406 Orsay Cedex (France)

Abstract. Some recent microscopic implementations of the particle-vibration coupling (PVC) theory for atomic nuclei are briefly reviewed. Within the nonrelativistic framework, the results seem to point to the necessity of fitting new effective interactions that can work beyond mean field. In keeping with this, the divergences which arise must be cured. A method is proposed, and the future perspectives that are opened are addressed.

1. Introduction
The fact that nucleons can be viewed as moving independently in an average potential, lies at the basis of the validity of self-consistent mean field (SCMF) models. These models, either in the nonrelativistic or covariant framework, are now rather sophisticated and produce good results for bulk nuclear properties like masses, radii, or the trends of deformations. A review of SCMF can be found in Ref. [1]. At the same time, the SCMF models do not account well for the single-particle spectroscopic data.

This fact can be considered to be consistent with the idea that SCMF is an implementation of the Density Functional Theory (DFT) for atomic nuclei, and single-particle states may not be within the DFT framework. However, the consequence is that we still lack a fully microscopic model that is able to describe single-particle properties along the isotopic table (in keeping with the limited applicability of ab-initio methods, and of the microscopic shell model). This issue has been recently addressed in Ref. [2].

In this reference, results for the single-particle states obtained from a recent implementation of the DFT are compared with those coming from the particle-vibration coupling (PVC) approach. In the case of PVC, results obtained within either a nonrelativistic or relativistic framework are discussed. PVC is supposed to take care of most of the dynamical correlations missing in the static SCMF models, in keeping with the fact that collective vibrations are the most important low-lying states of spherical nuclei. However, the conclusion of Ref. [2] is that it is hard to
extract a clear understanding why different theories predict different results - even in the case of a standard nucleus like $^{208}$Pb. Moreover, none of the theories is very accurate in reproducing the experimental data for the centroid (or main peak) of the single-particle strength distributions.

Experimentally, the single-particle strength displays also a non-negligible fragmentation, and theory should account for it. The fragmentation lies definitely outside the framework of DFT. This is perhaps the main motivation to try to generalize this framework, in which the basic variable is the static density, to a many-body theory where dynamical correlations are included. A simple version of this, is the PVC model (also called “dynamical” shell model). There are of course other motivations: for instance, the damping width of single-particle and collective states (like the nuclear giant resonances) can be described only by means of theories beyond SCMF or present day DFT.

If theories beyond mean field are necessary, we should expect to be obliged to re-fit at that level the effective forces that, so far, have been fitted at the mean field level. This has still to be done. The calculations discussed below, namely the recent implementations of PVC both in a nonrelativistic [3] and in a covariant [4] scheme, employ self-consistently the same interactions used for the mean field case like SLy5 or NL3.

In the case of zero-range forces, like the Skyrme interactions that have been used in Ref. [3] as well as in previous works, divergences arise when they are used beyond mean field. These divergences are associated with the use of a large model space. In the practical calculations, the model space is always truncated. For future applications, however, it is desirable to dispose of a regularization procedure.

A first step in this direction has been taken in Ref. [5]. In it, at least for a simplified Skyrme force applied to the case of uniform matter, it has been shown that the second-order divergence can be removed. In fact, for each upper cutoff in the model space, one can re-fit the interaction parameters so that the physical results are unchanged. The purpose of this contribution is to show these new results together, and discuss the perspectives that are open as a consequence.

2. Formalism of the particle-vibration coupling approach
Using standard many-body techniques, one can introduce the energy-dependent part $\Sigma(\omega)$ of the self-energy. It enters the well-known Dyson equation,

$$G(\omega) = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega),$$

that allows determining the Green’s function $G$ in terms of the unperturbed one $G_0$. In the present context, $G_0$ is the mean-field (i.e., Hartree-Fock) Green’s function. The $\Sigma(\omega)$ term is associated with the coupling to (mainly density) vibrations. We shall work in the so-called diagonal approximation, as defined in Ref. [6]: the quantities appearing in the Dyson equation (1) are written in the basis in which the mean-field is diagonal (that is, the HF basis), and only the diagonal matrix elements of $\Sigma(\omega)$ are considered. If the indices $i$, $p$ and $h$ label, respectively, a generic single-nucleon state, a particle state above the Fermi energy and a hole state below the Fermi energy, the diagonal matrix element $\Sigma_i$ reads

$$\Sigma_i(\omega) = \frac{1}{2j_i + 1} \left( \sum_{nL, p > F} \frac{|\langle i | |V| p, nL\rangle|^2}{\omega - \varepsilon_p - \omega_{nL} + i\eta} + \sum_{nL, h < F} \frac{|\langle i | |V| h, nL\rangle|^2}{\omega - \varepsilon_h + \omega_{nL} - i\eta} \right).$$

The energies $\omega_{nL}$ are the energies of the vibrational states (phonons) with angular momentum $L$, labeled by the index $n$. A (small) imaginary part $\eta$ is added in the denominators (it is set at 0.05 MeV in the calculations presented below). The numerators contain the squared modulus of a reduced matrix element called PVC vertex (see below).
The solution of the Dyson equation in the diagonal approximation is equivalent to the diagonalization of the matrix

$$
\begin{pmatrix}
\varepsilon_i & \langle i|V|k_1,n_1L_1 \rangle / \sqrt{2j_{i}+1} & \langle i|V|k_2,n_2L_2 \rangle / \sqrt{2j_{i}+1} & \cdots \\
\langle i|V|k_1,n_1L_1 \rangle / \sqrt{2j_{i}+1} & \varepsilon_{k_1} + \hbar \omega_{n_1L_1} & 0 & \cdots \\
\langle i|V|k_2,n_2L_2 \rangle / \sqrt{2j_{i}+1} & 0 & \varepsilon_{k_2} + \hbar \omega_{n_2L_2} & \cdots \\
\cdots & \cdots & \cdots & \cdots
\end{pmatrix}
$$

In this paper, we will show results obtained by using this method. They will be compared with those obtained by means of perturbation theory, that is, by calculating dressed single-particle energies defined by the equation

$$
\tilde{\varepsilon}_i = \varepsilon_i + \Sigma_i(\omega)|_{\omega=\varepsilon_i}.
$$

3. Results

Indeed, most of the calculations performed in the past have employed second-order perturbation theory, that is, Eq. (4). In the review paper [7], several calculations performed in the 80’s are compared and discussed. Qualitatively, they all demonstrate the relevance of the PVC to produce the single-particle strength fragmentation, as well as the increase of the level density (that is, the enhancement of the effective mass $m^*$) close to the Fermi energy which is empirically observed. However, none of them is consistent and it is hard to extract quantitative conclusions due to the many approximations involved.

Only recently, consistent calculations have been carried out. In the calculations presented below, based on the Skyrme interaction, first we solve the Hartree-Fock (HF) equations in coordinate space with the Skyrme parameter set SLy5 [8]. With the same parameter set we also perform fully self-consistent RPA calculations according to the formalism developed in Ref. [9, 10]. The interaction $V$ is the particle-hole interaction associated with the SLy5 functional. Both the velocity-dependent and velocity-independent parts are taken into account (only the residual two-body spin-orbit is dropped). All details, in particular the choice of the model space and the numerical parameters, are exactly as in Ref. [3], except for the fact that the perturbative expression was used there.

The results are shown in Table 1. They are compared with those obtained in Ref. [3] and the differences turn out to be small. In fact the r.m.s. difference between theory and experiment, which was quoted as 0.62 MeV in [3], is 0.59 MeV in the present work.

In Ref. [3], not only $^{40}$Ca but also $^{208}$Pb has been studied. In the latter case the r.m.s. between theory and experiment is 1.21 MeV: this number is obtained using perturbation theory, but we have seen that a full diagonalization is unlikely to change it significantly.

In the case of the relativistic mean field (RMF) plus PVC calculations of Ref. [4], the results seem qualitatively similar but quantitatively better. Perhaps this is due to the fact that the low-lying states display more collectivity in the case of the calculation of Ref. [4], than by employing the Skyrme set SLy5 of the present work. To check this point, new HF plus PVC calculations using one of the Skyrme sets that include tensor terms [13] (for instance using the set T44 that reproduces the values of the electromagnetic transition probabilities of the low-lying states within 10-20% [14]) should be envisaged. In any event, re-fitting the force would be certainly more satisfactory from a conceptual point of view.

4. The problem of the divergences beyond mean field

As recalled in the Introduction, the problem of re-fitting a Skyrme force by including contributions beyond mean field is hindered by the presence of divergences. Generally speaking,
Table 1. Results for the single-particle neutron energies in $^{40}$Ca, obtained within HF by employing the Skyrme force SLy5 (including the tensor force of Ref. [11] that has a negligible effect in this case), are shown in the second column. In the third and fourth columns we display the dressed single-particle energies obtained either from the perturbative formula (4), as in Ref. [3], or from the diagonalization of the matrix shown in Eq. (3). Finally, in the last column the experimental energies are shown (from Ref. [12]). All energies are in MeV.

| Energy Level | HF energies (SLy5 + tensor) | HF plus PVC perturbation theory | HF plus PVC diagonalization | Experimental energies |
|--------------|-----------------------------|-------------------------------|----------------------------|-----------------------|
| $1f_{5/2}$   | -1.26                       | -2.81                         | -2.64                      | -3.38                 |
| $2p_{1/2}$   | -3.11                       | -5.16                         | -4.93                      | -4.76                 |
| $2p_{3/2}$   | -5.28                       | -7.43                         | -7.17                      | -6.76                 |
| $1f_{7/2}$   | -9.69                       | -10.64                        | -10.55                     | -8.62                 |
| $1d_{3/2}$   | -15.17                      | -15.80                        | -15.76                     | -15.64                |
| $2s_{1/2}$   | -17.26                      | -18.32                        | -18.39                     | -18.19                |
| $1d_{5/2}$   | -22.10                      | -22.39                        | -22.37                     | -22.39                |

Figure 1. First- and second-order diagrams for the total energy in uniform fermionic matter. Labels refer to momentum states.

these divergences prevent from assessing unambiguously the results of calculations beyond mean field. Usually, these calculations are done by truncating the model space in some arbitrary way and this is by far an unsatisfactory procedure.

The self-energy of Eq. (2) belongs to the class of quantities that have an ultraviolet divergence in the case of a zero-range interaction. The same can be said for the corrections beyond mean field to the total energy or to other observables like the nuclear radius. Solving this problem is of general interest. Zero-range interactions are also employed for the study of dilute atomic gases [15]. In nuclear physics, the finite-range Gogny force has, nonetheless, a zero-range density-dependent term.

For all these reasons, the problem of ultraviolet divergences has been attacked in Ref. [5]. In this work, the zero-range interaction has been taken as a simplified Skyrme force with only velocity-independent $t_0$ and $t_3$ terms. We have studied the case of the second-order contributions to the total energy (see the bottom row of Fig. 1), in the case of a uniform Fermi system. A simple power counting argument shows the presence of the ultraviolet divergence. Whereas $k_1$ and $k_2$ are limited by the Fermi momentum $k_F$, $q$ can be arbitrarily large and for large values of this momentum transfer the second-order diagrams behave like

$$\sim \int d^3q \frac{v^2(q)}{q^2}. \quad (5)$$
For a zero-range force the matrix elements \( v \) are independent of \( q \) and a linear divergence shows up. In Ref. [5] the problem has been solved in the following way. The values of the second-order diagrams displayed in Fig. 1 have been calculated analytically as a function of the density \( \rho \) of the system, and of the upper limit of the \( \vec{q} \)-integral defined as \( \Lambda \) (the momentum cutoff). These second-order diagrams are found to provide a correction to the total energy \( \Delta E \) that can be written as

\[
\frac{\Delta E(\rho, \Lambda)}{A} = \chi(\rho) I(\rho, \Lambda).
\]  

(6)

\( A \) is the particle number, the value of \( \chi \) is

\[
\chi(\rho) = -\frac{3}{4\pi^6} \frac{mk^2_g}{\hbar^2 \rho},
\]  

(7)

where \( m \) is the fermion mass and \( g \) is the strength of the zero-range force \((g = t_0 + \frac{1}{6} \beta_3 \rho \alpha)\), and the divergent term reads

\[
I(\rho, \Lambda) = \frac{1}{105} (43 - 46 \ln 2) - \frac{18}{35} + \frac{\Lambda}{35k_F} + \frac{11\Lambda^3}{210k_F^3} + \frac{\Lambda^5}{840k_F^5} + \frac{16 \ln 2}{35}
\]

\[
+ \left( \frac{\Lambda^5}{60k_F^5} - \frac{\Lambda^7}{1680k_F^7} \right) \ln \left( \frac{\Lambda}{k_F} \right) + \left( \frac{1}{35} - \frac{\Lambda^2}{30k_F^2} + \frac{\Lambda^4}{48k_F^4} - \frac{\Lambda^6}{120k_F^6} + \frac{\Lambda^8}{3360k_F^8} \right) \ln \left( -2 + \frac{\Lambda}{k_F} \right)
\]

\[
- \left( \frac{1}{35} - \frac{\Lambda^2}{30k_F^2} + \frac{\Lambda^4}{48k_F^4} + \frac{\Lambda^6}{120k_F^6} - \frac{\Lambda^8}{3360k_F^8} \right) \ln \left( 2 + \frac{\Lambda}{k_F} \right).
\]  

(8)

By making appropriate expansions it is possible to show that this expression is linearly divergent for large values of \( \Lambda \), as expected from the above power counting argument.

The next step has been to include the momentum cutoff \( \Lambda \) among the parameters of the interaction, and to show numerically that for every value of \( \Lambda \) the remaining parameters \((t_0, t_3 \) and \( \alpha)\) can be determined in such a way that the total energy of the system remains always the same. Usually, the Skyrme forces are fitted so to reproduce the empirical saturation point of symmetric matter. We have assumed that the entire equation of state (EoS) of nuclear matter obtained with the Skyrme force SkP [16] at the mean field (HF) level, can be taken as a benchmark. This curve can be perfectly reproduced after including the second-order contributions to the energy, for every value of \( \Lambda \), by using the renormalized parameters (or, in other words, by adopting a renormalized interaction that can be labeled as SkP\( \Lambda \)). The good reproduction of the EoS can be viewed in Fig. 2, for different realistic values of \( \Lambda \).

The procedure discussed in this Section realizes the effective field theory (EFT) program in a simple, yet realistic case. Of course, the cutoff regularization might be replaced by other methods such as dimensional regularization if this turned out to be useful.

5. Conclusion

Although the success of mean field methods or, more generally, of DFT-based methods is undeniable, there exist situations where a many-body description in terms of dynamical quantities, like the Green’s function and the mass operator, is preferable. In nuclear physics, one of the most important dynamical processes that affect the single-particle properties is the coupling with low-lying, density vibrations. This is the rationale behind the well-known PVC theory. While in the past the PVC calculations contained uncontrolled approximations and phenomenological ingredients, microscopic PVC calculations are nowadays available. In this contribution, we have shown results of a recent Skyrme-HF implementation of PVC in the case...
Figure 2. Second-order-corrected equations of state compared with the reference equation of state (SkP at mean field level), for different values of the cutoff $\Lambda$.

of $^{40}$Ca, and compared in detail the energy of the neutron states obtained from perturbation theory and from matrix diagonalization. They are quite similar and in better agreement with experiment than the Skyrme-HF results.

At this stage, more systematic calculations should be envisaged, with the purpose of understanding to which extent the accuracy of PVC results can be improved, and whether higher order processes than those included in the PVC model of Sec. 2 are important. In any event, an effective force that has been fitted at the mean field level should be re-fitted when used beyond that level of approximation. In the case of zero-range forces, this is hindered by ultraviolet divergences.

We have shown in Sec. 4 that it is possible to develop strategies for the regularization of these divergences. We have indeed shown this explicitly in the case of the second-order contributions to the total energy in uniform symmetric matter. This paves the way to many new possible steps. Not only PVC models, but models where 2 particle-2 hole, or $n$ particle-$n$ hole couplings with zero-range forces are introduced, can benefit from further refinements of our technique. Using zero-range forces also the RPA correlation energy diverges; one should be able, eventually, to cure this divergence as well.

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