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Nuclear single-particle states: dynamical shell model and energy density functional methods

P.F. Bortignon^{1,2}, G. Colò^{1,2}, and H. Sagawa³

¹ Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, Milano, Italy

² Istituto Nazionale di Fisica Nucleare (INFN), Sez. di Milano, via Celoria 16, Milano, Italy

³ Center for Mathematics and Physics, University of Aizu, Aizu-Wakamatsu, Fukushima 965-8560, Japan

E-mail: bortignon@mi.infn.it, colo@mi.infn.it, sagawa@u-aizu.ac.jp

Abstract. We discuss different approaches to the problem of reproducing the observed features of nuclear single-particle spectra. In particular, we analyze the dominant energy peaks, and the single-particle strength fragmentation, using the example of neutron states in ^{208}Pb . Our main emphasis is the interpretation of that fragmentation as due to particle-vibration coupling (PVC). We compare with recent Energy Density Functional (EDF) approaches, and try to present a critical perspective.

1. Introduction

One of the most striking features of nuclei is the validity of the shell model where the nucleons move independently in a smooth single-particle (s.p.) potential. However, self-consistent mean field (SCMF) approaches [1] are much more successful in reproducing the bulk properties that emerge from the mean field picture (like masses, that can nowadays be reproduced by Skyrme-HFB calculations with a remarkable accuracy of about 0.6 MeV [2]) than in accounting for the s.p. states.

If SCMF is viewed as an approximate realization of an exact, yet unknown and perhaps unfeasible, Density Functional Theory (DFT), it is not surprising that quantities like the total energy are well accounted for since they belong to the domain of this theory based on the well-known Kohn-Sham theorem. (We do not enter here the problem if this theorem can be expected to hold in a self-bound system since this discussion can be found elsewhere in the present volume).

If single-particle states are not, strictly speaking, within the DFT framework, two possible routes can be undertaken. Some authors [3, 4, 5, 6] are currently trying to improve the accuracy of present DFT implementations aiming at functionals with so-called “spectroscopic” accuracy (referring to, of course, single-particle spectroscopy). Another point of view, which is the preferred one by the authors of the present contribution, is to generalize the shell model to the so-called “dynamical” shell model

[7, 8, 9, 10]. It has to be noted that the former attitude does not solve the problem of evaluating the so-called spectroscopic factors or, more generally, the well-known fragmentation of the s.p. strength.

The potential emerging from SCMF calculations is static, but in general nonlocal in space (or, in equivalent words, velocity- or momentum-dependent). The fluctuations of this average potential lead to collective modes, in particular surface vibrations. Taking into account the coupling of these modes to the s.p. motion, the shell model acquires a dynamical content. Thus, the average potential becomes also nonlocal in time, being characterized by an energy (or frequency) dependence.

The velocity dependence of the s.p. potential can be characterized by the so-called k -mass m_k , and its frequency dependence by the ω -mass m_ω [7]. Most experiments only probe the product of these two quantities, that is, the “total” effective mass m^* (see the definitions in Sec. 2). The dynamics of the shell model affects different nuclear properties as: the fragmentation and related spectroscopic factors of the s.p. states, their density (which is proportional to m^* near the Fermi energy), the s.p. spreading widths, and the imaginary component of the optical potential. A unified description of the s.p. motion at positive and negative energy eventually emerges.

The importance of the dynamical couplings was first demonstrated in the case of electrons in metals and of normal liquid ^3He . These results inspired the work of Bertsch and Kuo [11] on the enhancement of the effective mass near the Fermi energy in finite nuclei. The review article [7] contains the formalism reported in the next Section as well as the many results obtained in the 80s. The expression “dynamics of the shell model” is after G.E. Brown [12].

The old calculations of the 80s are mostly not consistent. It is hard to extract quantitative conclusions because of the many approximations involved. More consistent calculations have been recently done. They can be confronted with modern EDF-based approaches. We shall do it in the simple case of ^{208}Pb , showing that the problem of the s.p. states is still an open one.

2. Formalism of the dynamical shell model

One can introduce using standard many-body techniques a “mass operator” \mathcal{M} , defined by (see, e.g., Ref. [7])

$$[\omega + (2m)^{-1}\nabla_r^2] G(\vec{r}, \vec{r}'; \omega) = \delta(\vec{r} - \vec{r}') + \int d_3r' \mathcal{M}(\vec{r}, \vec{r}'; \omega) G(\vec{r}, \vec{r}'; \omega) \quad (1)$$

in terms of the one-body Green function (Lehmann representation)

$$G(\vec{r}, \vec{r}'; \omega) = \sum_h \frac{\phi_h(\vec{r}) \phi_h^*(\vec{r}')}{\omega - \omega_h - i\eta} + \sum_p \frac{\phi_p(\vec{r}) \phi_p^*(\vec{r}')}{\omega - \omega_p + i\eta}. \quad (2)$$

Here

$$\begin{aligned} \phi_h(\vec{r}) &= \langle \psi_h^{(A-1)} | a(\vec{r}) | \psi_0^{(A)} \rangle, \\ \phi_p(\vec{r}) &= \langle \psi_0^{(A)} | a(\vec{r}) | \psi_p^{(A+1)} \rangle. \end{aligned} \quad (3)$$

$\psi_h^{(A-1)}$ is a suitably normalized eigenstate of the Hamiltonian of the (A-1)-particle system with energy $E_h^{(A-1)}$, $\psi_p^{(A+1)}$ is a suitably normalized eigenstate of the Hamiltonian of the (A+1)-particle system with energy $E_p^{(A+1)}$, and

$$\omega_p = E_p^{(A+1)} - E_0^{(A)} \quad \omega_h = E_0^{(A)} - E_h^{(A-1)}. \quad (4)$$

Eqs. (1) and (2) give

$$[\omega + (2m)^{-1}\nabla^2] \phi_p(\vec{r}) - \int d_3r' \mathcal{M}(\vec{r}, \vec{r}'; \omega_p) \phi_p(\vec{r}') = 0. \quad (5)$$

This s.p. wave equation has two important properties: i) It has discrete eigenvalues corresponding to the energies of the bound states of the (A+1) and (A-1) systems, ii) In the continuum gives the exact diagonal (elastic scattering) element of the S matrix [13].

The mass operator, in what follows, will contain the Hartree-Fock (HF) mean field and the contribution of the coupling of the s.p. HF states to the vibrational modes (particle-vibration coupling or PVC), in particular to collective modes obtained from self-consistent linear response theory (Random Phase Approximation or RPA).

Although one could solve (5) directly, the usual way has been so far to solve it at the HF level and add the contribution of the particle-vibration part of the mass operator within second-order perturbation theory. The expressions for this second-order correction can be found, e.g., in Refs. [7, 8].

To work out the expressions for m_k , m_ω and m^* , it is easier to consider a uniform system [7]. Thus, having the relation

$$E = \frac{k^2}{2m} + \mathcal{V}(k; E) \quad (6)$$

between the energy E and the momentum k of the quasiparticle (dressed s.p.), and \mathcal{V} being the real part of the complex mass operator, the effective mass is defined

$$\frac{dE}{dk} = \frac{k}{m^*}. \quad (7)$$

Then, it is easy to write

$$\begin{aligned} \frac{m_k}{m} &= \left\{ 1 + \frac{m}{k} \left[\frac{\partial \mathcal{V}(k; \omega)}{\partial k} \right] \right\}_{\omega=E(k)}^{-1}, \\ \frac{m_\omega}{m} &= 1 - \left[\frac{\partial}{\partial \omega} \mathcal{V}(k; \omega) \right]_{\omega=E(k)}, \end{aligned} \quad (8)$$

to obtain

$$\frac{m^*}{m} = \frac{m_k}{m} \cdot \frac{m_\omega}{m}. \quad (9)$$

3. The contradicting results

3.1. Particle-vibration coupling: old and new results

In Tables 4.3a and 4.3b of Ref. [7], an extensive review of the results obtained for m_ω in ^{208}Pb by nine groups in the period 1968-1983 can be found. Rather different frameworks

had been adopted, no one being fully self-consistent: s.p. potentials range from harmonic oscillator (HO) to Woods-Saxon (WS) or HF with Skyrme forces; residual interactions at the particle-vibration vertex are either multipole-multipole forces, or forces of Landau-Migdal type, or Skyrme forces but with velocity-dependent terms dropped, or even G-matrix interactions.

The average value for m_ω is in the range 1.2-1.4 for the neutron valence shells, and in the range 1.3-1.6 for the proton case. The inverse of m_ω gives the spectroscopic factor reported in table 4.4 of Ref. [7]. In general, it has been impossible to find an accurate agreement between theory and experiment, either at the level of main energy centroids of the s.p. strength distribution, or at the level of spectroscopic factors. The problem of spectroscopic factors had been not considered too seriously, in view of the large experimental errors and ambiguities associated with them. Nowadays, new analysis are being carried out [14], but the theoretical ambiguities associated with the extraction of spectroscopic factors are still under discussion (see e.g. the contribution by R. J. Furnstahl and A. Schwenk in the present volume).

If we concentrate on s.p. energies, the most consistent among the calculations reported in [7], namely that by V. Bernard and N. Van Giai [8], still underestimates the density of levels.

Table 1. Shifts (that, is differences between dressed and bare single-particle energies) associated with the dominant s.p. neutron components in ^{208}Pb . See the text for a discussion of how they have been obtained.

	$\Delta\varepsilon = \varepsilon_i - \varepsilon_i^{(0)}$		
	[9]	[10]	[3]
3d _{3/2}	-0.61	-0.32	0.09
4s _{1/2}	-0.56	-0.21	0.24
3d _{5/2}	-0.76	-0.43	0.07
1j _{15/2}	-1.36	-0.55	
2g _{9/2}	-0.79	-0.40	0.03
1i _{11/2}	-0.31	-0.37	-0.14
3p _{1/2}	-0.02	0.01	0.05
2f _{5/2}	0.33	0.01	0.12
3p _{3/2}	0.14	0.03	0.06
1i _{13/2}	0.49	0.05	0.22
1h _{9/2}	1.40	0.06	
2f _{7/2}	1.40	0.63	0.12

The most recent calculations for ^{208}Pb in the framework of dynamical shell model, or PVC model, have been reported in Refs. [9] and [10]. The results are displayed in Tables 1 and 2 and compared with the results of Ref. [3] (cf. below) and with the experimental energies, in the case of the neutron valence particle and hole states. In Table 1 we display, for Refs. [9] and [10], the differences between the s.p. energies ε_i obtained with PVC included, and the mean field energies $\varepsilon_i^{(0)}$. These differences $\Delta\varepsilon_i$ will be called “shifts” in what follows. (See below for a definition of the shifts from Ref.

[3]).

In the covariant theory of Ref. [9], the mean field is associated with the NL3 [15] effective Lagrangian, which is also employed to obtain the phonons within the relativistic RPA (RRPA). The Dyson equation (2) for the s.p. Green's functions is solved in the diagonal approximation for the mass operator \mathcal{M} . A rather simple particle-vibration model is used, in which the coupling vertex is obtained with the matrix element of the residual interaction times the transition density of the vibrations.

The calculations of Ref. [10] are performed in the framework of Skyrme HF, with the PVC contributions to the mass operator \mathcal{M} calculated within second-order perturbation theory. The phonons are obtained through fully self-consistent RPA, and all the terms of the particle-hole (p-h) interaction are kept also in the PVC vertex. There are strong cancellations due to the velocity dependent terms that lead to small shifts, especially for the hole states. The calculations have been done using the SLy5 Skyrme set [16]. Calculations with other Skyrme functionals are in progress.

Table 2. Dressed single-particle energies and spectroscopic factors S associated with the dominant s.p. neutron components in ^{208}Pb , compared with the experimental findings.

	ε_{th}			ε_{exp}	S_{th}		S_{exp}
	[9]	[10]	[3]		[9]	[10]	
3d _{3/2}	-0.63	0.01	0.78	-1.40	0.89	0.94	0.88±0.1
4s _{1/2}	-0.92	-0.31	0.80	-1.90	0.92	0.95	0.88±0.1
3d _{5/2}	-1.39	-1.08	-0.43	-2.37	0.88	0.91	0.88±0.1
1j _{15/2}	-1.84	-1.75		-2.51	0.66	0.86	0.53±0.1
2g _{9/2}	-3.29	-3.62	-3.16	-3.94	0.84	0.93	0.78±0.1
1i _{11/2}	-3.28	-1.38	-1.67	-3.16	0.88	0.94	0.96±0.2
3p _{1/2}	-7.68	-8.04	-8.06	-7.37	0.90	0.93	1.07
2f _{5/2}	-8.77	-8.94	-8.91	-7.94	0.86	0.94	1.13
3p _{3/2}	-8.27	-9.16	-9.17	-8.27	0.86	0.91	1.00
1i _{13/2}	-9.11	-10.13	-9.30	-9.00	0.81	0.94	1.04
1h _{9/2}	-11.96	-12.01		-10.78	0.36	0.94	1.10
2f _{7/2}	-9.71	-11.44	-11.90	-9.71	0.64	0.75	0.88

In Ref. [3], the HF problem is solved for the even-even and even-odd ($A\pm 1$) systems using the SLy4_L interaction. The “dressed” energies ε_i are obtained from an equation like the present Eq. (4). In this case E_0 is the total energy of the even-even system and E_p (E_h) is the total energy of the odd system when a given occupancy (vacancy) is imposed. The “bare” energies are obtained by excluding the so-called mass, shape and spin polarization effects: in practice this corresponds, respectively, to neglecting the proper change of the center-of-mass correction, to imposing spherical symmetry, and to discarding time-odd terms.

One can see from Table 1 that shifts obtained by RMF plus PVC and Skyrme plus PVC are different, and it is hard to connect either of them to the calculations of [3]. If we look now at the final “dressed” energies obtained in the different approaches (Table

2), and compare with experimental values, we conclude that the open problem is that even for the “benchmark” nucleus ^{208}Pb we do not dispose of a consistent calculation which reproduces well the experimental data. This is also true for spectroscopic factors.

In the calculations of the spectroscopic factors, the effects of the short-range correlations (SRC) should also be included. On the one side, in a recent work [17], it is confirmed that the PVC involving long-range correlations (LRC) can be identified as the main mechanism, the SRC explaining only a small fraction (up to about 10%) of the deviations of the spectroscopic factors from the independent s.p. values. Consistently, from a qualitative point of view, in Ref. [7] it was concluded that the main contribution of highly excited core polarized states to m_ω , and therefore to the spectroscopic factors, can be considered as a constant in the vicinity of the Fermi energy. The subtracted dispersion relation technique, with different choices for the behaviour of the imaginary part of the mass operator at high energy, was used.

3.2. EDF extensions

The lack of an accurate description of s.p. states is also clear for EDF practitioners not only in keeping with the findings of Ref. [3]. The authors of [4] have concluded that standard forms of the Skyrme energy density functional do not allow that accurate description. The effect of tensor forces has been studied very carefully by the authors of [18, 19], but their conclusion is that the tensor terms, albeit important, cannot remedy the deficiencies of the central terms: in practice, they cannot produce a functional which is more accurate as far as s.p. states are concerned.

In Ref. [5], gradient corrections up to next-to-next-to-next-to-leading order (N^3LO , in practice derivatives up to sixth power) have been added to a local EDF, in order to better reproduce surface effects, for example on the effective mass m_ω (cf. also [20]). The precision on s.p. states is improving [6].

4. Conclusions

We still lack, despite the tremendous progress in many aspects of nuclear structure physics, an accurate description of s.p. strength distributions. While new radioactive beam facilities have already started to show how this kind of observables evolve with the decrease of the neutron or proton separation energies [21, 22], even for standard nuclei we have troubles to get accuracy for dominant s.p. energies and spectroscopic factors (using models that have had big success in reproducing other kind of observables).

The addition of higher power gradient corrections to a local EDF may improve the s.p. energies. We deem, however, that a dynamical theory is necessary to describe quantities like the spectroscopic factors. The merging of the two approaches defines anyway, to some extent, the future of this fundamental field of nuclear structure research. In a many-body approach like the dynamical shell model one believes that the basic object should be a time- or energy-dependent quantity like the s.p. Green’s function.

EDF practitioners aiming at functionals with spectroscopic accuracy believe that a static approximation, in which the Green's function reduces to a static density, may be a sound approximation. This issue asks for a clear answer based on comparison of results without uncontrolled approximations.

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