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Correlations Beyond Mean Field Based on Covariant Density Functional Theory*

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Abstract. The concept of Density Functional Theory (DFT) is a mapping of the complicated quantum mechanical many-body problem to a one-body problem, which can be solved relatively easily. Correlations are taken into account by the violation of symmetries. There are, however, cases, where this mechanism is not sufficient, and where one has to go beyond mean field. There are extensions of nuclear density functional theory which start from successful phenomenological nuclear density functionals and allow, without new parameters, the mixing of configurations and the description of excited states. We give an overview of such methods for covariant density functional theory and discuss a number of recent applications, such as the treatment of complex spectra in transitional nuclei or the coupling of single particle motion to collective phonons.

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1 Introduction

In recent years microscopic descriptions starting with the bare nucleon-nucleon forces have made essential progress in describing the properties of light and even specific medium heavy nuclei. Still, even now, the largest part of the nuclear chart is only accessible to mean field calculations, i.e. to density functional theory (DFT). Indeed modern nuclear density functionals provide a very complete description of ground-state properties and specific collective excitations all over the periodic table. In principle DFT presents a mapping of the complicated nuclear many-body problem to a self-consistent single particle problem, which can be solved easily on modern computers, even for complicated finite range density functionals or for heavy and super-heavy nuclei of all kinds of shapes and far from the valley of β-stability [1, 2] However, so far, all these successful

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functionals dependent on phenomenological parameters adjusted to specific nuclear data. At present, all attempts to derive these functionals directly from the bare forces do not reach the required accuracy [3].

One of the underlying symmetries of QCD is Lorentz invariance and therefore covariant density functional theory (CDFT) [4–6] is of particular interest in nuclear physics. This theory exploits basic properties of QCD at low energies, in particular, symmetries and the separation of scales [2]. It provides a consistent treatment of the spin degrees of freedom, and includes the complicated interplay between the large Lorentz scalar and vector self-energies which are induced on the QCD level by inmedium scalar and vector quark condensates [7]. It also includes nuclear currents caused by the spatial parts of the vector self-energies, which play an essential role for magnetic moments [8] and in rotating nuclei [9].

In principle, according to the Hohenberg-Kohn theorem [10], density functional theory should be exact in Coulombic systems [11]. Whether this is also true in self-bound systems such as nuclei, is still a question under debate [12]. On the other side nuclear DFTs can incorporate short-range correlations related to the repulsive core of the inter-nucleon interaction. In the sense of Brueckner theory [3], this leads to density dependent interactions. Therefore short-range correlations are incorporated in nuclear DFT in a phenomenological way. Many of the long-range correlations, as for instance the important quadrupole correlations, are included by symmetry breaking. Indeed, a deformed single particle model, such as the Nilsson model [13] provides an excellent description of a tremendous number of data, whereas spherical single particle models are not able to describe the level density at the Fermi surface and the fragmentation of single particle excitations.

A mean field description of nuclei, such as DFT suffers from three essential shortcomings:

(i) the symmetry violation, which provides the possibility to include long-range correlations, leads to wave functions without good quantum numbers, which are necessary for a successful description of spectroscopic data,

(ii) in many cases, such as in transitional nuclei, the nuclear wave function cannot be described properly by a single Slater determinant with a fixed deformation. One observes shape-coexistence [14] with several minima in the energy surface. One also finds often very flat energy surfaces, where quantum fluctuations in the deformation have to be taken into account by configuration mixing,

(iii) in spherical nuclei with closed shells, one finds in nearly all mean field theories a much too low level density at the Fermi surface, which means a low effective mass, and sometimes strongly fragmented single particle excitations.

In this contribution we discuss methods to include long range correlations in covariant DFT theories. In Section 2 we use configuration mixing in the framework of the generator coordinate method (GCM) for deformed and transitional nuclei

and in Section 3 we describe the treatment of correlations in spherical nuclei by particle-vibrational coupling which leads to energy dependent self energies.

2 Symmetry Restoration and Configuration Mixing in Deformation Space

In covariant density functional theory, we start from the functional

$$E[\rho,\kappa] = E_{\rm RMF}[\rho] + E_{\rm pair}[\kappa] \tag{1}$$

where $E_{\rm RMF}[\rho]$ corresponds to a relativistic mean field (RMF) model and $E_{\rm pair}[\kappa]$ is the pairing energy. For reasons of numerical simplicity in all the practical applications one has used in this context point-coupling models, such as DD-PC1 [15] or PC-PK1 [16].

Starting from this functional the constrained relativistic Hartree-Bogoliubov (RHB) equations [17] are solved in the BCS approximation for a grid of mesh points in deformation space $q = (\beta, \gamma)$ such that for given collective coordinates q the expectation values of the quadrupole operators are given by

$$\langle \hat{Q}_{20} \rangle = \frac{3}{4\pi} R^2 \beta \cos\gamma, \qquad \langle \hat{Q}_{22} \rangle = \frac{3}{4\pi} R^2 \frac{1}{\sqrt{2}} \beta \sin\gamma \tag{2}$$

GCM is based on the assumption that, starting from a set of intrinsic symmetry-breaking states $|\Phi(q)\rangle$ one can build approximate eigenstates of the nuclear Hamiltonian with good angular momentum quantum numbers I, M and good particle numbers N and Z for neutrons and protons

$$\left|\Psi^{I(\alpha)}_{M}\right\rangle = \sum_{Kq} f^{(\alpha)}_{K}(q)\, \hat{P}^{I}_{MK} \hat{P}^{N} \hat{P}^{Z} \, |\Phi(q)\rangle \ . \tag{3}$$

where $\hat{P}^{I}_{MK}$, $\hat{P}^{N}$, and $\hat{P}^{Z}$ are projection operators onto good angular momentum and the number of neutrons and protons (for detail see Refs. [18, 19]).

Integration in the 7-dimensional GCM-state in Eq. (3) is performed over the three Euler angles in the angular momentum projectors, the two gauge angles for neutron and protons and the deformation parameters $q = (\beta, \gamma)$. The weight functions $f^{(\alpha)}_{K}(q)$ are determined from the variation,

$$\delta E^{I} = \delta \frac{\langle \Psi^{I(\alpha)}_{M} | \hat{H} | \Psi^{I(\alpha)}_{M} \rangle}{\langle \Psi^{I(\alpha)}_{M} | \Psi^{I(\alpha)}_{M} \rangle} = 0 \ , \tag{4}$$

i.e. by requiring that the expectation value of the energy is stationary with respect to an arbitrary variation $\delta f^{I(\alpha)}_{K}$. This leads to the Hill-Wheeler equation [20] for the unknown functions $f^{(\alpha)}_{K}(q)$,

$$\sum_{Kq'} \mathcal{H}^{I}_{MK}(q,q') f^{I(\alpha)}_{K}(q') = E^{I\alpha} \sum_{Kq'} \mathcal{N}^{I}_{MK}(q,q') f^{I(\alpha)}_{K}(q') \ , \tag{5}$$

with the kernels

$$\mathcal{H}^I_{MK}(q,q') = \langle\Phi(q)|\hat{H}\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi(q')\rangle \quad (6)$$
$$\mathcal{N}^I_{MK}(q,q') = \langle\Phi(q)|\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi(q')\rangle \quad (7)$$

The Hill-Wheeler equation (5) presents a generalized eigenvalue problem. Its solution involves a considerable numerical effort, even for medium heavy nuclei, but with increasing computer power there are more and more with non-relativistic Skyrme [21–26] and Gogny [27–31] forces and with covariant density functionals [32–35] For large scale and systematic investigations, however, additional approximations have been considered, as for instance the Gaussian Overlap Approximation (GOA) [18] one assumes that for large particle numbers the overlap functions

$$\langle\Phi(q)|\hat{H}|\Phi(q')\rangle \quad \text{and} \quad \langle\Phi(q)|\Phi(q')\rangle \quad (8)$$

fall off sharply in the form of a Gaussian in $(q-q')$. A similar approximation is used for the angular momentum projection where the collective coordinates are the three Euler angles Ω. An expansion up to second order in the momenta [36] leads to a second order differential equation in the deformation coordinates and the Euler angles. This is a Schrödinger equation with the collective Hamilton operator of the Bohr model [37]. Formally this can be expressed as

$$\left[\frac{\hbar^2}{2}\frac{\partial}{\partial q}\frac{1}{B(q)}\frac{\partial}{\partial q} + V(q)\right] f(q) = Ef(q) \quad (9)$$

where

$$V(q) = \langle\Phi(q)|\hat{H}|\Phi(q)\rangle + V_{\text{corr}}(q) \quad (10)$$

is the potential energy surface with additional correction terms. The inertia parameters $B(q)$ derived from the GCM-ansatz are the Yoccoz inertia [38] parameters. They do not reproduce the exact mass in the case of translations. Therefore, in practical applications, they are usually replaced by the Cranking approximation, i.e., in the case of rotations, by the Inglis-Belyaev formula [39] or, in rare cases, by the Thouless-Valatin inertia [40].

Obviously this method is fully microscopic. All the parameters of the five-dimensional collective Hamiltonian in the two deformation variables β and γ and the three Euler angles are derived from the original energy density functional. In practice the calculations are relatively simple, because one only has to calculate the potential and the inertia parameters as a function of q and one avoids the complicated overlap functions (8).

In Figure 1 we show an application of these methods to the spectrum of the transitional nucleus ^{76}Kr. The CDFT-parameter set PC-PK1 [16] is used here and we compare the experimental (a) data with results of the full seven-dimensional GCM-calculation (b) and the approximate solution based on the Bohr-Hamiltonian

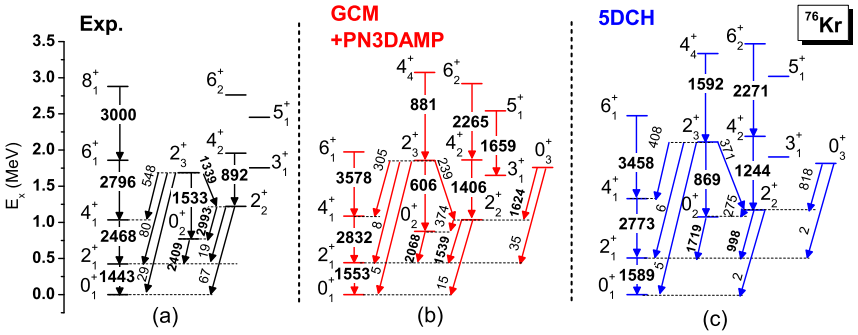

Figure 1. Low-lying spectra and B(E2) values (in e^2 fm^4) of ^{76}Kr. Experimental results (a) are compared with (b) full relativistic GCM results with number and three dimensional angular momentum projection and with (c) 5DCH results. This figure is reprinted with permission from [41]. Copyright American Physical Society 2014.

in five dimensions (5DCH). We find excellent agreement for this complicated spectrum with a ground state band, a quasi-β-band and a very disturbed quasi-γ-band. This shows that the assumptions of the GOA are justified already for this medium heavy nucleus and gives a clear justification of the use of a collective Hamiltonian. Therefore this method is nowadays used in many relativistic [42–45] and non-relativistic [46–50] applications

3 Correlations in Spherical Nuclei

A mean field description of nuclei with closed shells, in particular of doubly magic nuclei leads to spherical configurations. Therefore quadrupole and other long range correlations are not included. Since Bohr and Mottelson [37] and Landau-Migdal theory [52] it is well known, that one can include in this case correlations by the coupling of the single particle motion to low-lying collective excitations. In order to describe such collective vibrations in the framework of a density functional theory one has to go beyond the mean field approximation.

This can be done by time-dependent density functional theory [53,54]. According to the Runge-Gross theorem [55], for a given initial condition, the exact single particle density $\rho(\boldsymbol{r},t)$ of a quantum-mechanical many-body problem in a time-dependent external single potential $f_{ext}(\boldsymbol{r},t)$, can be expressed in terms of time-dependent single particle wave functions ϕ_i, $\rho(\boldsymbol{r},t) = \sum_i^N |\phi_i(\boldsymbol{r},t)|^2$ The ϕ_i's obey a time-dependent Kohn-Sham equation

$$i\partial_t\phi_i(\boldsymbol{r},t) = \left[-\nabla^2/2m + v[\rho(\boldsymbol{r},t)]\right]\phi_i(\boldsymbol{r},t), \tag{11}$$

where the Kohn-Sham potential $v[\rho(\boldsymbol{r},t)]$ is a unique functional of the time-dependent density $\rho(\boldsymbol{r},t)$. In order to calculate it at a given time t_1 it is not enough to have the density $\rho(\boldsymbol{r},t_1)$ at that time, but one has to know the entire

history $\rho(\boldsymbol{r},t)$. As a consequence the derivation would require the full solution of the exact Schrödinger equation for arbitrary systems with the density $\rho(\boldsymbol{r},t)$, i.e. memory effects have to be included. This is of course very complicated and in practice one considers only weak external fields such that the motion is close to the static solution, where we can use our knowledge about the static density functional. In linear order one finds for the changes of the density

$$\delta\rho(\boldsymbol{r},t) = \int d^3r' \int dt' R(\boldsymbol{r},\boldsymbol{r}',t-t') f_{ext}(\boldsymbol{r}',t'). \tag{12}$$

and after a Fourier transformation in t the response function $R(\boldsymbol{r},\boldsymbol{r}',\omega)$ obeys the linear response equation [18]

$$\begin{aligned} R(\boldsymbol{r},\boldsymbol{r}',\omega) &= R_0(\boldsymbol{r},\boldsymbol{r}',\omega) \\ &\quad + \int d^3r_1 d^3r_2 R_0(\boldsymbol{r},\boldsymbol{r}_1,\omega) V(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega) R(\boldsymbol{r}_2,\boldsymbol{r}',\omega) \end{aligned} \tag{13}$$

Here the interaction is in principle the functional derivative of the time-dependent Kohn-Sham potential $v[\rho(\boldsymbol{r},t)]$ with respect to the density at the static value. Since we do not know this functional, we use the adiabatic approximation,

$$v[\rho(\boldsymbol{r},t)] \approx v_s[\rho_t(\boldsymbol{r})] \tag{14}$$

treating t only as a parameter and replacing the functional $v[\rho(\boldsymbol{r},t)]$, which depends on a function of four variables, by the static functional $v_s[\rho_t(\boldsymbol{r})]$ depending only on a function of three variables using the density at that time. In this case the effective interaction in Eq. (13) does not depend on time and we find

$$V(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{\delta^2 E[\rho]}{\delta\rho(\boldsymbol{r}_1)\delta\rho(\boldsymbol{r}_2)} \tag{15}$$

In this approximation the linear response equation (13) corresponds to the small amplitude limit of time-dependent mean-field theory, the well known random phase approximation (RPA) [18]. Its solution leads to all kind of collective and non-collective excitations $|\mu\rangle$ of ph-type, low-lying surface vibrations, giant resonances, and so on.

In the next step we go back to the time-dependent Kohn-Sham equation (11) and construct a model for the complicated functional $v[\rho(\boldsymbol{r},t)]$, which couples the single-particle motion to the collective vibrations, the solutions of the RPA.

In a relativistic many-body theory the motion of single nucleons in the nuclear medium is described by the Dyson equation

$$\big(\gamma^\mu(p_\mu + \Sigma_\mu)P_\mu - (m+\Sigma_s)\big)|\psi\rangle = 0, \tag{16}$$

with the scalar and vector self-energies Σ_s and $(\Sigma_0, \boldsymbol{\Sigma})$.

For the ground sate this self energy corresponds to the static Kohn-Sham potential in the Dirac equation and it is derived from the static energy density functional. We therefore assume in the following that at low energies this momentum and energy-dependence is small and can be treated in a linearized approximation. We therefore decompose all the components of the total self-energy in a stationary local part $\tilde{\Sigma}(\mathbf{r})$ and an energy-dependent non-local term

$$\Sigma(\mathbf{r},\mathbf{r}';\omega) = \tilde{\Sigma}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') + \Sigma^e(\mathbf{r},\mathbf{r}';\omega). \tag{17}$$

$\tilde{\Sigma}$ corresponds to the static RMF fields in the Dirac hamiltonian h_D and we find the stationary Dirac equation

$$\big(h_D + \Sigma^e(\varepsilon)\big)|\psi\rangle = \varepsilon|\psi\rangle. \tag{18}$$

Obviously, on this stage one needs some model assumptions. The particle-phonon coupling model [37] provides a rather simple approximation to describe the energy dependence of $\Sigma^e(\varepsilon)$. The main assumption of this model is that two types of elementary excitations – $1p1h$ states and low-lying vibrational modes (phonons) – are coupled in such a way that configurations of $1p1h \otimes phonon$ type strongly compete with simple $1p1h$ configurations close in energy or, in other words, that particles can emit and absorb phonons with rather high probabilities. In this way a fully consistent description of the many-body dynamics is obtained. In Figure 2 we show the corresponding diagrams for the relativistic case. Since the self-energy $\Sigma^e(\varepsilon)$ depends on energy, the resulting single particle levels are fragmented, as it is observed in experiment. Each fragment has a certain spectroscopic factor.

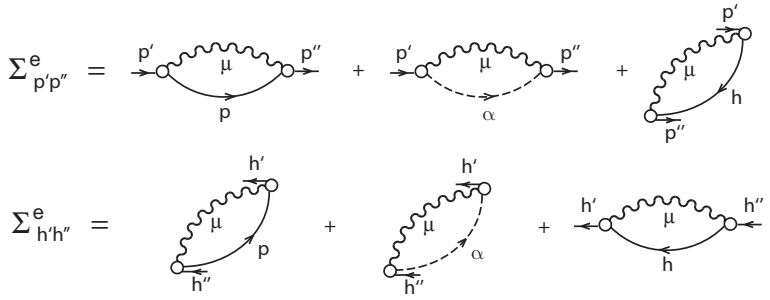

Figure 2. Graphical representation of the energy dependent parts of the relativistic self-energy for particles $\Sigma^e_{p'p''}$ and holes $\Sigma^e_{h'h''}$. This figure is reprinted with permission from [51]. Copyright American Physical Society 2007.

To illustrate the resulting shifts in the level schemes, we show in Figure 3 the dominant poles for the neutrons in ^{208}Pb. They are compared with the RMF results and the experimental data. The spectrum calculated with the energy-dependent correction (RMF+PVC) demonstrates a pronounced increase of the

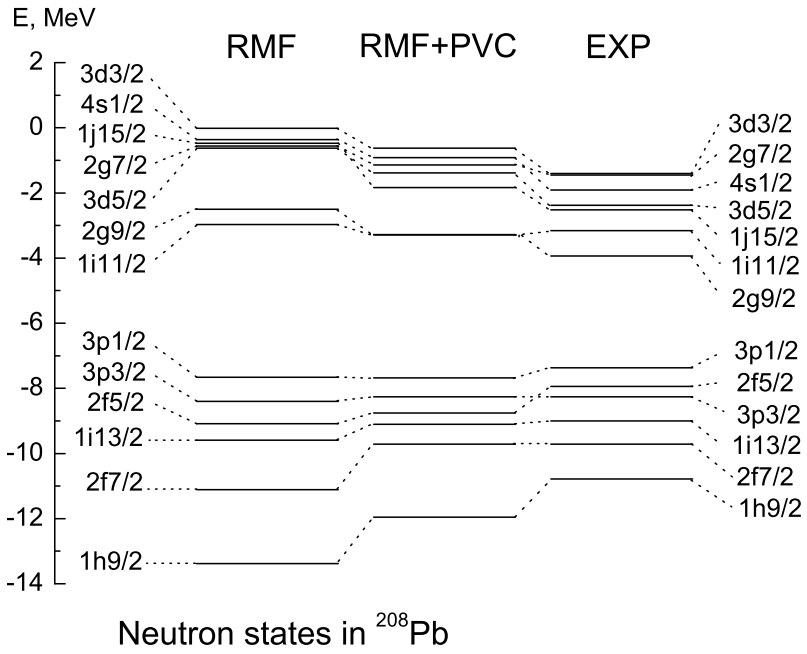

Figure 3. Neutron single-particle states in ^{208}Pb: the pure RMF spectrum (left column) is compared with results from a consistent particle-vibration coupling (center) and with experimental data (right). This figure is reprinted with permission from [56]. Copyright American Physical Society 2006.

level density around the Fermi surface compared to the pure RMF spectra. In some cases the order of levels is inverted and the observed sequence is reproduced as for instance for the $1j_{15/2}$ and the $3d_{5/2}$ neutron states. Another and more important example is the inversion of the $2g_{9/2}$ and $1i_{11/2}$ neutron states which reproduces the spin of the ^{209}Pb ground state. Similar investigations have been carried out in the non-relativistic case in the framework of Landau-Migdal theory of Finite Fermi Systems [57,58], in Nuclear Field Theory [59,60], and in self-consistent density functional theory based on Skyrme forces [61].

Based on the energy-dependent self energy of Eq. (18) we can go a step further and determine the energy dependence in the effective interaction in the response equation (13) by a derivative of $\Sigma(\varepsilon)$ with respect to ρ. This leads in the relativistic quasiparticle time-blocking approximation (RQTBA) to an induced interaction in the form of a phonon exchange (for details see Ref. [51]). and a fragmentation of the giant resonance spectrum including complex configurations such as $2p-2h$-excitations and to a considerable increasing of the width. In Figure 4 we show applications in the Sn-region which are in good agreement with the experiment.

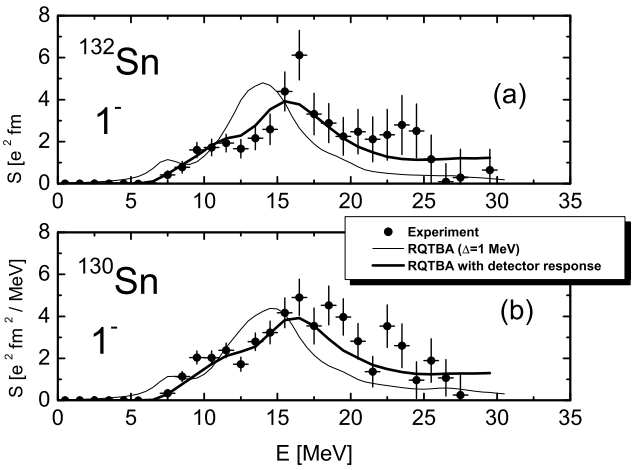

Figure 4. Spectra of dipole excitations in ^{130}Sn, ^{132}Sn. RQTBA results with 1 MeV smearing are compared with experimental data [62]. The thick curves are obtained after the convolution with the detector response. This figure is reprinted with permission from [63]. Copyright American Physical Society 2009.

4 Conclusions

Covariant density functional theory is a powerful tool for the description of ground state properties of nuclei all over the nuclear chart. Correlations are taken into account on the mean field level by symmetry breaking. It is however limited to cases which can be treated within the mean field approximation. We gave an overview over methods to overcome this problem. They all start with the same Lagrangian, but they apply additional configuration mixing. In deformed systems this can be done by linear combination of various product states in the framework of GCM, which allows to restore symmetries and to take into account fluctuations. The numerical effort is tremendous and therefore we discussed the derivation of a collective Bohr hamiltonian that allows fast applications with excellent results.

In spherical nuclei additional correlations are taken into account in the framework of time-dependent density functional theory. It leads to an energy dependent interaction which allows to couple to more complex configurations. In the small amplitude limit and with the help of techniques developed in the framework of Fermi liquid theory for finite systems the phonons and all the necessary interactions can be derived from the same static energy density functional. We discussed applications beyond mean field that overcome problems, such the low level density at the Fermi surface and the reduced width of giant resonances. Such methods can, in principle, also be applied in deformed systems. However, fully consistent applications have to wait for the future.

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