Covariant density functional theory with spectroscopic properties and a microscopic theory of quantum phase transitions in nuclei.

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Abstract. Covariant Density functional theory is used as a basis for a microscopic description of spectroscopic properties of quantum phase transitions in nuclei. Since it is well known that the mean field approximation breaks down in transitional nuclei, where configuration mixing and fluctuations connected with broken symmetries play an important role, a theory is developed which uses the Relativistic Generator Coordinate Method to perform configuration mixing calculations of angular momentum and particle number projected wave functions. As applications with show 3D-calculations of the spectrum of low-lying collective states in the nucleus \textsuperscript{24}Mg. This method can also be used to study the behavior of characteristic physical quantities as a function of the physical control parameter, the number of nucleons, in the region of quantum phase transitions.

1. Introduction

Theoretical approaches based on Covariant Density Functional Theory (CDFT) remain undoubtedly among the most successful microscopic descriptions of nuclear structure. The CDFT approaches are derived from a Lorentz invariant density functional which connects in a consistent way the spin and spatial degrees of freedom in the nucleus. Therefore, it needs only a relatively small number of parameters which are adjusted to reproduce a set of bulk properties of spherical closed-shell nuclei [1, 2] and it is valid over the entire periodic table. Over the years, Relativistic Mean-Field (RMF) models based on the CDFT have been successfully applied to describe ground state properties of finite spherical and deformed nuclei over the entire nuclear chart [3] from light nuclei [4] to super-heavy elements [5, 6], from the neutron drip line where halo phenomena are observed [7], to the proton drip line [8] with nuclei unstable against the emission of protons [9]. The relativistic cranking approximation has been developed to calculate rotational bands [10, 11]. For a description of nuclear excited states, the Relativistic Random Phase Approximation (RRPA) [12] and the quasiparticle RRPA (RQRPA) [13] have been formulated as the small amplitude limit of the time-dependent RMF models. These models
have provided a very good description for the positions of giant resonances and a theoretical interpretation of the low-lying dipole [13] and quadrupole [14, 15] excitations. Proton-neutron versions of the RRPA and the RQRPA have been developed and successfully applied to the description of spin/isospin excitations as the Isobaric Analog Resonance (IAR) or the Gamow-Teller Resonance (GTR) [16].

This framework has, however, its limitations. It is based on the mean-field concept which is characterized by symmetry breaking and can only provide an approximate description of specific nuclear excitations, such as collective rotations in the framework of the Cranking model or vibrations in the framework of time-dependent mean field theory, which corresponds in the small amplitude limit to RPA or QRPA. To calculate excitation spectra with specific quantum numbers and electromagnetic transition rates in individual nuclei, it is necessary to extend this framework to include collective correlations related to the restoration of broken symmetries and to fluctuations of collective coordinates. Collective correlations are sensitive to shell effects, display pronounced variations with particle number, and cannot be incorporated in a single Slater determinant.

On this level density functional theory takes into account collective correlations through the restoration of broken symmetries and configuration mixing of symmetry-breaking product states. In recent years several accurate and efficient models and algorithms have been developed that perform the restoration of symmetries broken by the static nuclear mean field, and take into account fluctuations around the mean-field minimum. The most effective approach to configuration mixing calculations is the generator coordinate method (GCM) [17, 18]. With the simplifying assumption of axial symmetry, GCM configuration mixing of angular-momentum, and even particle-number projected quadrupole-deformed mean-field states, has become a standard tool in nuclear structure studies with non-relativistic [19, 20], and relativistic density functionals [21, 22].

Much more involved and technically difficult is the description of intrinsic quadrupole modes including triaxial deformations. Only very recently fully microscopic three-dimensional calculations have been presented for Skyrme [23] and Gogny [24] mean field models generated by triaxial quadrupole constraints that are projected and mixed by the generator coordinate method. This method is actually equivalent to a seven-dimensional GCM calculation, mixing all five degrees of freedom of the quadrupole operator and the gauge angles for protons and neutrons. Here we report on configuration mixing of angular-momentum projected triaxial relativistic mean-field wave functions based on covariant density functionals [25].

2. The relativistic generator coordinate method.
The generator coordinate method is based on the assumption that, starting from a set of mean-field states $|\Phi(q)\rangle$ which depend on collective coordinates $q$, one can build approximate eigenstates of the nuclear Hamiltonian by linear combination of such states:

$$|\Psi_\alpha\rangle = \int dq f_\alpha(q) |\Phi(q)\rangle \ .$$

Detailed discussions of the GCM method can be found in Ref. [17]. To be able to compare theoretical predictions with data, it is necessary to construct states with good angular momentum

$$|\Psi^{JM}_\alpha\rangle = \int dq \sum_{K \geq 0} f^{JM}_\alpha(q) \frac{1}{(1 + \delta_{K0})} |JM K+, q\rangle$$

$\alpha$ labels collective eigenstates for a given angular momentum $J$. The details of the 3D angular-momentum projection in the relativistic case are given in Ref. [26]. The basis states $|JM K+, q\rangle$
are projected from the intrinsic wave functions $|\Phi(q)\rangle$:

$$|JMK+, q\rangle = [\hat{P}_{MK}^J + (-1)^J \hat{P}^J_{M-K}]|\Phi(q)\rangle,$$

where $\hat{P}_{MK}^J$ is the angular-momentum projection operator.

The set of intrinsic wave functions $|\Phi(q)\rangle$, with the generic notation for quadrupole deformation parameters $q \equiv (\beta, \gamma)$, is generated by imposing constraints on the axial $q_{20}$ and triaxial $q_{22}$ mass quadrupole moments in self-consistent RMF+BCS calculations. The following calculations are based on the relativistic point coupling model PC-F1 [27]. Pairing correlations are taken into account in the simple BCS approximation, using a $\delta$-pairing force.

![Figure 1](image_url)

Figure 1. (Color online) Self-consistent RMF+BCS energy surface (left panel) of $^{24}$Mg in the $\beta-\gamma$ plane ($0 \leq \gamma \leq 60^0$), and angular momentum projected energy surface with $J^\pi = 0^+$ (right panel). The contours join points on the surface with the same energy. The difference between neighboring contours is 1.0 MeV.

The weight functions $f_{\alpha K}(q)$ in the collective wave function Eq. (2) are determined from the variation of the energy by the Hill-Wheeler-Griffin (HWG) integral equation:

$$\int dq' \sum_{K' \geq 0} \left[ \mathcal{H}_{K'K}(q, q') - E_{\alpha K'} \mathcal{N}_{K'K}(q, q') \right] f_{\alpha K}(q') = 0,$$

where $\mathcal{H}$ and $\mathcal{N}$ are the angular-momentum projected GCM kernel matrices of the Hamiltonian and the norm, respectively.

As an example for an illustrative configuration mixing calculation we investigate the spectrum of the nucleus $^{24}$Mg. The intrinsic wave functions have been obtained as solutions of the self-consistent relativistic mean-field equations, subject to constraint on the triaxial mass quadrupole moments.

Fig. 1 shows the self-consistent RMF+BCS triaxial energy surface in the $\beta-\gamma$ plane. The panel on the right displays the projected energy surface with $J = 0$. The energy surfaces nicely illustrate the effects of including triaxial shapes and of the restoration of rotational symmetry. The mean-field energy surfaces are found to be quite soft with a minimum at an axial prolate deformation $\beta = 0.5$. Projection shifts the minimum to a triaxial shape with $\beta = 0.5$ and $\gamma = 0.20^0$. The gain in energy from the restoration of rotational symmetry is 4.266 MeV. The fact that angular momentum projection leads to triaxial minima in the PES was already been
noted in 3DAMP calculations in the eighties [31] and very similar results have been obtained recently using the Skyrme functional SLy4 [23].

Fig. 2 displays the spectrum of the nucleus $^{24}\text{Mg}$, calculated with the 3DAMP+GCM and 1DAMP+GCM codes. The 3DAMP+GCM and 1DAMP+GCM calculations produce virtually identical results. The level scheme is in rather good agreement with data, but in both cases the calculated spectra are systematically stretched as compared to experimental bands. This is because angular-momentum projection is performed only after variation and, therefore, time-odd components and alignment effects are neglected. Cranking calculations, for instance, correspond to an approximate angular-momentum projection before variation [32], and lead to an enhancement of the moments of inertia in better agreement with data [11, 33]. The agreement of the calculated quadrupole transition probabilities with data in Fig. 2 is remarkable, especially considering that the calculation of $B(E2)$ values is parameter-free, i.e. the transitions are calculated employing bare proton charges.

The nucleus $^{24}\text{Mg}$ presents an illustrative test case for the 3DAMP+GCM approach to low-energy nuclear structure. However, collective phenomena are, of course, much more pronounced in heavy nuclei and, therefore, the goal is to eventually apply the present approach to rare earth nuclei and the actinide region. At present a straightforward application of the existing 3DAMP+GCM codes to heavy nuclei is not possible. On the other hand, the introduction of additional approximations can considerably reduce the computing requirements. For instance, the overlap functions are strongly peaked at $q = q'$, and the use of the Gaussian overlap approximation has produced excellent results in many cases. These approximations form the basis for a microscopic derivation of a collective Bohr Hamiltonian for quadrupole degrees of freedom [34, 35] based on covariant density functionals.

3. A microscopic theory of quantum phase transitions

Quantum phase transitions from spherical to deformed shapes have recently gained considerable interest. However, most of these investigations have carried out within simple boson models [37]. The Generator Coordinate Method has recently been applied for a microscopic theory of quantum phase transitions in finite nuclei. Starting from constrained self-consistent mean-field calculations of potential energy curves, the one-dimensional generator coordinate
method (GCM) is used to perform configuration mixing of angular-momentum and particle-number projected relativistic wave functions [38]. It is shown that the microscopic framework based on universal density functionals, adjusted to nuclear ground-state properties and extended to take into account correlations related to symmetry restoration and fluctuations of collective variables, describes not only general features of shape transitions but also the unique behavior of excitation spectra and transition rates at the critical point of quantum shape phase transition. In particular the shape phase transition occurs precisely at the isotope $^{150}$Nd, in agreement with empirical evidence for the realization of X(5) in the $N = 90$ rare-earth isotones. As shown in Fig. 3 the calculated spectrum and the intra-band and inter-band B(E2) transitions for $^{150}$Nd are in excellent agreement with data [36] and close to the X(5)-model predictions for the nucleus $^{150}$Nd [37].

Because of the considerable numerical effort 3D angular momentum projected GCM calculations are at present not yet possible for such heavy nuclei as the Ne-chain. Therefore this phase transition has been investigated recently [39] on the basis of a 5-dimensional Bohr hamiltonian, whose parameters were derived microscopically form the covariant density functional PC-F1. The resulting spectrum and the electromagnetic transition probabilities are more or less the same as in the 1D-AMP GCM calculation shown in Fig. 3.

4. Summary and outlook.
Among the microscopic approaches to the nuclear many-body problem, the framework of nuclear density functional theory provides the most complete description of ground-state properties and collective excitations over the whole nuclide chart. The self-consistent mean-field models based on the density functional framework describe not only general features of shape transitions but also particular properties of spectra and transition rates at the critical point of the QPT.

Figure 3. The particle-number projected GCM spectrum of $^{150}$Ne (left), compared with the data [36] (middle), and the X(5)-symmetry predictions (right) for the excitation energies, and B(E2) values (in Weisskopf units) of the ground-state and the $\beta$-band. The theoretical spectra are normalized to the experimental energy of the state $2^+_1$, and the X(5) transition strengths are normalized to the experimental B(E2; $2^+_1 \rightarrow 0^+_1$).

5
However, to calculate excitation spectra and transition probabilities, the self-consistent mean-field approach has to be extended to include correlations related to restoration of broken symmetries and fluctuations of collective variables. This can be done either by performing GCM configuration mixing calculations of projected wave functions or by constructing collective Bohr-type Hamiltonians with deformation-dependent parameters determined from self-consistent mean-field calculations. The possibility to perform self-consistent microscopic studies of shape transitions opens a new perspective on the origin of nuclear quantum phase transitions in various mass regions. It is therefore important to systematically analyze these methods, also employing different energy-density functionals, various types of shape phase transitions that have been predicted in several regions of medium-heavy and heavy nuclei.

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