Quasiparticle-vibration coupling in relativistic framework: shell structure of $Z=120$ isotopes

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Abstract

For the first time, the shell structure of open-shell nuclei is described in a fully self-consistent extension of the covariant energy density functional theory. The approach implies quasiparticle-vibration coupling for superfluid systems. One-body Dyson equation formulated in the doubled quasiparticle space of Dirac spinors is solved for nucleonic propagators in tin isotopes which represent the reference case: the obtained energies of the single-quasiparticle levels and their spectroscopic amplitudes are in agreement with data. The model is applied to describe the shell evolution in a chain of superheavy isotopes $^{292,296,300,304,120}$ and finds a rather stable proton spherical shell closure at $Z=120$. An interplay of the pairing correlations and the quasiparticle-phonon coupling gives rise for a smooth evolution of the neutron shell gap between $N=172$ and $N=184$ neutron numbers. Vibrational corrections to the alpha decay energies reach several hundred keV and can be either positive and negative, thus also smearing the shell effects.
Impressive progress of experimental low-energy nuclear physics such as synthesis of many exotic nuclei \cite{1}, superheavy nuclei \cite{2-4} and discovering new nuclear structure phenomena \cite{5} insistently calls for conceptually new theoretical methods. High-precision description of nuclear properties still remains a challenge for contemporary theoretical physics. Besides describing the experimentally known phenomena, theory has to make predictions to guide future experimental searches and to model physical situations which are not yet available in laboratories, but occur in the astrophysical conditions.

One of the most promising strategies for medium-mass and heavy nuclei is the construction of a "universal" nuclear energy density functional \cite{6} supplemented by various many-body correlations. The existing and commonly used concepts do not yet allow a high-precision description of nuclear properties due to their very limited or not self-consistent treatment of many-body correlations. However, such a reliable description is urgently needed for fast progressing disciplines like nuclear astrophysics or synthesis of superheavy elements. Delicate interplay of different kinds of correlations is responsible for binding loosely-bound systems, decay properties and for low-energy spectra.

Our recent attempts to extend the covariant energy density functional (CEDF) approach use the relativistic framework \cite{7,8} in combination with advancements of the Landau-Migdal theory for Fermi liquids in parameter-free quantum field theory techniques \cite{9-11}. Couplings of single-particle and collective degrees of freedom are included far beyond the standard mean field and random phase approximations in a fully self-consistent way. On top of the CEDF these techniques turned out to be very successful in the description of nuclear low-energy dynamics even for exotic very neutron-rich nuclei \cite{10-14}. The considerable success of these self-consistent many-body methods shows that they (i) represent the right strategy towards a universal and precise approach and (ii) already allow exploration of experimentally unknown regions of the nuclear chart: nuclei with exotic neutron to proton (N/Z) ratios and superheavy nuclei.

In the approaches based on the density functional concept, single-particle properties such as energies and spectroscopic amplitudes are the key ingredients for a description of nuclear masses, decay properties and responses to diverse external fields. In turn, the latter quantities are an essential part of the nuclear physics input for astrophysical applications like r-process nucleosynthesis studies \cite{15} which require the information about many nuclei including exotic ones. It has been found recently that shell structure in nuclei with extreme
N/Z ratios deviates from the usual picture and magic numbers are shown to change as functions of N and Z [16].

The shell structure of superheavy nuclei is another challenge for microscopic models: to define the location of spherical shell gaps in this area of the nuclear chart is necessary to determine the regions of stability of these nuclei. Up to now, there is no consensus about the spherical shell closures above the proton Z = 82 and neutron N = 126 ones: predictions such as Z = 114, Z = 120 or Z = 126 for the proton and N = 172 or N = 184 for the neutron magic numbers can be found in the literature [17, 18]. The Z = 120 and N = 172 shell closures predicted by the relativistic and some Skyrme mean-field models are found to be related to a central depression of the nuclear density distribution [17, 19]. The Z = 120 element represents a challenge for future experimental synthesis since it is located at the limits of accessibility with available cold fusion reactions. Therefore, accurate estimations of its characteristics are needed from the theoretical side.

The predictions made by the mean field models, however, ignore correlations which can play a significant role in the superheavy mass region where the expected spherical shell gaps are considerably smaller (2-3 MeV) than in lighter nuclei and pairing correlations of the superfluid type may not collapse at the shell closures. It has been found in Ref. [14] that superheavy nuclei are very soft objects: they possess very rich spectra of low-lying collective vibrations (phonons). Therefore, correlations due to the quasiparticle-vibration coupling (QVC) are then the next important mechanism having considerable influence on the shell structure.

Medium-mass and heavy nuclei represent Fermi-systems where single-particle and vibrational degrees of freedom are strongly coupled. Collective vibrations lead to shape oscillations of the mean nuclear potential and, therefore, modify the single-particle motion. To take this effect into account, already in Ref. [20] a general concept for the phonon coupling part of the single-nucleon self-energy has been proposed. This concept has had diverse implementations over the years [9, 14, 21, 26], however, these studies either are not self-consistent or do not include pairing correlations of the superfluid type. In this Letter a fully self-consistent model, implementing both superfluid and vibrational correlations in the relativistic framework, is formulated and applied to a description of single-quasiparticle spectra of tin and Z=120 isotopes.

Single-particle degrees of freedom in nuclei are characterized by the single-(quasi)particle
energies and the spectroscopic amplitudes which can be determined in one-nucleon transfer or knockout reactions. In microscopic many-body models these quantities enter the well known Lehmann expansion of the one-body Green’s function of the N-body system over the eigenstates of the N±1-body systems:

\[ G(\xi, \xi'; \varepsilon) = \sum_n \frac{(\bar{\Psi}(\xi))_{m0}(\bar{\Psi}(\xi'))_{n0}}{\varepsilon - (E^{(N+1)}_n - E^{(N)}_0) + i\delta} + \sum_m \frac{(\bar{\Psi}(\xi'))_{m0}(\bar{\Psi}(\xi))_{n0}}{\varepsilon + (E^{(N-1)}_m - E^{(N)}_0) - i\delta}, \]

where \(\delta \rightarrow +0\), \(\Phi^{(N)}_0\), \(\Phi^{(N)}_n\) are the many-body wave functions of the ground and the excited state \(n\) of the N-body system, \(E^{(N)}_0\), \(E^{(N)}_n\) are its ground state and excited state energies, and the variable \(\xi\) includes the full set of the single-particle variables in an arbitrary representation. The numerators of Eq. (1) give the spectroscopic amplitudes of the states \(n\). To calculate these spectroscopic amplitudes and the corresponding energies, the Dyson equation is solved with a one-body Hamiltonian that consists of a Relativistic Hartree-Bogoliubov (RHB) part \(H_{RHB}\) and an additional energy-dependent self-energy \(\Sigma^{(e)}(\varepsilon)\):

\[ (\varepsilon - H_{RHB} - \Sigma^{(e)}(\varepsilon))G(\varepsilon) = 1. \]

In the present work the space of the Dirac spinors diagonalizing the RHB Hamiltonian is taken as a working basis. In this case \(\xi = \{k, \eta\}\), where \(k\) is the full set of the single-particle quantum numbers in the spherical relativistic mean field (RMF) and \(\eta = \pm 1\) denotes the upper and lower components in the Bogoliubov’s quasiparticle space. Thus, the entities in the Eq. (3) are supermatrices in this space:

\[ \sum_{\eta=\pm 1} \sum_k \left((\varepsilon - \eta_1 E_k)\delta_{\eta_1 \eta_2}^\eta \delta_{k_1 k_2} - \sum_{k_1 k_2} \Sigma^{(e)}_{k_1 k_2}(\varepsilon)\right)G^\eta_{k k_2}(\varepsilon) = \delta_{\eta_1 \eta_2}^\eta \delta_{k_1 k_2}. \]

Here \(E_k\) are the eigenvalues of the RHB hamiltonian and \(\Sigma^{(e)}_{k_1 k_2}(\varepsilon)\) is the nucleonic self-energy of the quasiparticle-phonon coupling:

\[ \Sigma^{(e)}_{k_1 k_2}(\varepsilon) = \sum_{\eta=\pm 1} \sum_{k, \mu} \frac{\gamma_{\mu k k_1}^\eta \gamma_{\mu k k_2}^{\eta^*}}{\varepsilon - \eta (E_k + \Omega_\mu - i\delta)}. \]

The index \(\mu\) labels the set of vibrational modes taken into account and \(\Omega_\mu\) are their frequencies computed with the relativistic quasiparticle random phase approximation (RQRPA). The vertices \(\gamma\) determine the coupling of the quasiparticles to the vibrational modes.
FIG. 1: (Color online) Single-quasiparticle spectrum of $^{116}$Sn: RMF (left column), QVC (center) and experimental data (right). In the 'QVC' and 'EXP' cases only the dominant levels are shown.

In spherical nuclei, the self-energy $\langle \gamma \rangle$ has very small off-diagonal matrix elements, thus the Green's function $G(\epsilon)$ is supposed to be diagonal. Solutions of the Eq. (4) provide the quasi-particle energies and the strength distributions (spectroscopic factors) $S_n(\xi) = |\langle \psi(\xi) \rangle_n|^2$.

Before applying the model to unknown nuclei, benchmarking calculations have been done for nuclei which had been investigated experimentally. Tin isotopes represent a very good reference case as their single-quasiparticle energies and spectroscopic factors in the vicinity of the Fermi energy (FE) are known [28]. The neutron and proton single-quasiparticle levels in $^{116}$Sn and $^{120}$Sn are shown in Figs. 1 and 2. In each panel, the left columns display the mean-field energies of the Bogoliubov quasiparticles, the columns in the middle represent the dominant levels (levels with the largest spectroscopic strength $S_n(\xi)$) obtained within the QVC model and on the right the experimentally observed dominant levels are shown.

In the applications to the doubly-magic nuclei [9, 14], as a rule, the QVC correlations push the dominant levels towards the FE. However, for the states, which are very close to the FE, the QVC shift effect on the dominant levels is rather weak. In open-shell neutron subsystems of $^{116,120}$Sn, where the FE is in the middle of the shell, there are several states of this kind.
Because of the relatively high level density inside the valence shell, the leading terms in the sum of Eq. (5) may compensate each other. In contrast, in the closed-shell proton subsystems the level density at the FE is smaller, thus, there are weaker compensations and the shifts are considerably larger. For all dominant levels in $^{116,120}$Sn nuclei one can find a very good agreement of the presented QVC results with the data. The obtained spectroscopic factors reproduce the available data also very well: their detailed analysis will be presented elsewhere. The success of the response theory built on the nucleonic self-energy of Eq. (5) [10] can be now traced back to the results of the present work showing that for a proper description of nuclear shell structure and dynamics both types of correlations – pairing and quasiparticle-vibration coupling – should be taken into account self-consistently on the equal footing.

The $^{292,296,300,304}^{120}$ isotopes have spherical minima of the potential energy surfaces in both Skyrme and CEDF calculations [29], therefore, it is justified to keep spherical symmetry for their mean-field potentials. The newest non-linear meson-exchange interaction NL3* [30] used for the CEDF in this work is the slightly improved NL3 one [31] known to give a very good agreement with data for various low-energy phenomena not only in medium-mass nuclei, but also in $A\approx$250 mass region [32] and, therefore, it is justified to use this parameter.
FIG. 3: (Color online) Single-quasiparticle strength distribution for the orbits around the Fermi surfaces in the neutron (left panels) and proton (right panels) subsystems of the Z=120 isotopes calculated in the relativistic quasiparticle-vibration coupling model. The dashed lines indicate the chemical potentials.

set for the superheavy systems as well as for the tin isotopes. The Bardeen-Cooper-Schrieffer model for pairing correlations as well as the HFB model lead to a collapsing solution in the Z=120 proton subsystem so that pairing correlations can be restored only by approximate particle number projection methods [33]. In the neutron subsystems, however, no pairing collapse is found for Z = 120 nuclei, thus, in the present work pairing has been included for the neutrons. In the superheavy mass region the shell gaps are considerably smaller than those between the previous shells. They amount about 2-3 Mev and, therefore, are compatible with non-vanishing neutron pairing which, in turn, slightly increases the gaps. The phonon spectra calculated with the RQRPA in the chain of Z=120 isotopes show that these nuclei are very soft: many rather collective phonons with \( J^\pi = 2^+, 3^-, 4^+, 5^-, 6^+ \) are found below 15 Mev and included into the self-energy [5].

The selected results on the single-quasiparticle strength distributions in the neutron and
TABLE I: Alpha decay energies [MeV] for even-even Z=120 isotopes with N = 176-184 calculated in the covariant density functional theory without (RMF) and with (RMF+VC) vibrational corrections.

| N   | 176 | 178 | 180 | 182 | 184 |
|-----|-----|-----|-----|-----|-----|
| RMF | 11.81 | 11.55 | 11.28 | 11.23 | 11.60 |
| RMF+VC | 11.73 | 11.68 | 11.65 | 11.41 | 11.91 |

The proton subsystems of the Z = 120 isotopic chain are displayed in Fig. 3. The distributions for the orbits closest to the neutron and the proton FE’s are given and denoted by different colors. Thus, one can see the evolution of these distributions with an increase of the neutron number from N = 172 to N = 184. As in the neutron subsystems both pairing and QVC mechanisms are included, their very delicate interplay is found: pairing correlations tend to increase the shell gap while the QVC tends to decrease it and at the same time causes the fragmentation of the states in the middle of the shell. As a result, in the presence of both mechanisms the gap in the neutron subsystem remains almost steady while the newly occupied levels jump down over the gap when the neutrons are added. The shell gap in the proton subsystems of the considered nuclei diminishes only slightly when the neutron number increases, so that the proton number Z = 120 remains a rather stable shell closure while the detailed structure of the proton levels shows some rearrangements induced by the neutron addition.

The zero-point fluctuations associated with the nuclear vibrational motion affect the nuclear binding energies [34, 35]. This effect is especially important for the superheavy alpha-emitters as their lifetimes are related directly to the differences of the binding energies of the mother and the daughter nuclei. In order to obtain the correct nuclear binding energy, the vibrational correlations should be, in principle, incorporated into the fitting procedure for the underlying energy density functional [35]. However, for the differential quantities like alpha decay energies the vibrational corrections (VC) can be performed after the minimization procedure. For all the considered Z = 120 isotopes the RQRPA vibrational corrections to the total energies amount 4-5 MeV being comparable to the shell correction energies. Alpha decay energies for the even-even Z=120 isotopes calculated within the RMF and the RMF+VC models are displayed in Table I. One can see that the vibrational corrections to
the alpha decay energies reach several hundred keV and can be both positive and negative introducing either stabilizing or destabilizing effect. As a result, the lifetime predictions change correspondingly: in the case of the largest VC in $^{300}_{120}$, the decrease of the lifetime of this nucleus is up to an order of magnitude, depending on the evaluation method [36].

In conclusion, the relativistic quasiparticle-vibration coupling model is formulated. The results obtained for the experimentally known nuclei illustrate that the self-consistent implementation of many-body correlations beyond the CEDF represents a successful strategy towards a universal and precise approach for the low-energy nuclear dynamics. The model has allowed looking deep inside the shell structure of $Z = 120$ isotopes representing hypothetically an island of stability for superheavy nuclei. It has been found that the proton number $Z = 120$ remains a rather stable spherical shell closure when the neutron number changes from $N = 172$ to $N = 184$. In the neutron subsystem, due to an interplay of pairing and quasiparticle-vibration coupling, the smooth evolution of the shell structure is observed, so that at all the neutron numbers $N = 172, 176, 180, 184$ comparable spherical shell gaps are found. The analysis of the alpha decay energies has included, for the first time, the vibrational corrections and shown that these corrections can amount several hundred keV in both directions smearing the irregularities due to the shell effects.

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