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Density functional theory for reactions of astrophysical interest

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ABSTRACT

For astrophysical processes nuclear reactions close to the particle emission threshold are of particular importance. As representative examples we investigate pairing resonances and new low-energy multipole modes in light and heavy exotic nuclei with a large charge asymmetry. As a common theoretical background, density functional theory and Fermi Liquid Theory are used. In particular, we consider the spectroscopy particle unstable systems, carrying the properties of open quantum systems. Results for the continuum spectroscopy of ¹⁰Li, the neutron-rich carbon isotopes, and the electromagnetic response of Sn-isotopes ¹³⁸Ba are presented.

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1. Introduction

The description of nucleo-synthesis on a quantitative level is still a challenge. Beside the fact that the astrophysical sites of nucleo-synthesis are still not unambiguously identified there are also remaining uncertainties with respect to the nuclear physics input. From the point of view of nuclear theory, nuclear reactions in weakly bound nuclei and close to the particle threshold are of interest by themselves. These are processes which occur typically under extreme conditions concerning the charge-to-mass ratio. Hence, isospin effects are tremendously magnified, much beyond any level known from particle stable nuclei close to the valley of stability. The energy scales, set by the separation energies of valence particles, are changed drastically from about $S \sim 10$ MeV in $N \sim Z$ nuclei to $S \sim 100$ keV in nuclei close to the proton and neutron driplines. This reduction by a factor of 100 or more has important consequences for the dynamics in those systems. While in stable nuclei the nucleonic motion is dominated by mean-field dynamics, i.e., stationary states in a static potential, this concept comes to its limits in exotic nuclei: there, level spacings and separation energies are of the order of the matrix elements of residual interactions. This implies that the mean-field loses its dominant role and we have to expect that collision processes among nucleons will be enhanced significantly and contribute increasingly to the binding energy of such nuclei. This also implies that shell structures will be resolved because their existences rely completely on the presence of a common static potential. Therefore, a new ordering of levels has to be expected at the extremes. However, hitherto it is an open question where exactly the limits of mean-field dynamics are located. It could be very well that this question can be decided locally, i.e., the type of dynamics might depend strongly on the mass and charge region.

Weakly bound and particle unstable, unbound nuclei are of a new quality. Under a very general point of view, they carry the properties of open quantum systems. In other fields of physics open quantum systems are well established and well studied. In nuclear physics, however, the huge separation energies in stable nuclei allowed to neglect to a large extent the cross-talk between the spectral region of bound and continuum states. Therefore, the traditional approach of nuclear manybody theory is based on an almost strict separation between nuclear structure physics, mainly concerned with the spectral properties of bound systems, and nuclear reaction physics, being responsible for investigations of scattering processes of



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various kinds between nuclei. For nuclear physics, it is a new experience that this division might no longer hold and should be reconsidered in favor of a more general, unified approach to nuclear dynamics.

As a common theoretical basis for both sectors of nuclear physics we choose the nuclear density functional theory. The theoretical aspects are discussed in Section 2. In Section 3 the continuum spectroscopy in light neutron-rich nuclei is discussed, in Section 4 we consider low-energy multipole excitations in heavy nuclei. In Section 5 the paper closes with a summary and an outlook.

2. Nuclear density functional theory

In many cases, nuclear reactions of astrophysical interest involve nuclei with exotic charge-to-mass ratios. Such systems are located close to or at the driplines, typically characterized by small separation energies of the excess nucleons. An important consequence is that the clear separation of the bound, discrete and the unbound, continuous parts of the spectra are no longer meaningful. In order to account for this new feature, appropriate theoretical methods must be developed. The continuum shell model and related methods are promising approaches, also allowing, in principle, an *ab initio* description. However, having in mind investigations over large mass regions, not restricted to light elements, proper extensions of the density functional theory (DFT) and the related mean-field methods are worthwhile alternatives. Using a formulation based on nucleon field operators Ψ_q for protons (q = p) and neutrons (q = n), respectively, the single particle continua are fully included. Denoting discrete quantum numbers except energy and linear momentum by α , the field operators are given by:

$$\Psi_q = \sum_{q\alpha} \left(\sum_n a^+_{q\alpha n} \psi_{q\alpha n} + \int \frac{\mathrm{d}^3 k}{(2\pi)^3} c^+_{q\alpha k} \chi_{q\alpha k} \right) \tag{1}$$

where we explicitly distinguish operators and wave functions belonging to the discrete part $(a_{\alpha n}^+, \psi_{\alpha n})$, and the continuous part, $(c_{\alpha q}^+, \chi_{\alpha q})$, of the spectrum, respectively. Corresponding expressions hold for the hermitian conjugate field operator $\Psi^{\dagger} \equiv \overline{\Psi}$. Since we are only interest in virtual meson exchange processes in the t- and the u-channels, we eliminate the meson fields ϕ_m in favor of the meson (Yukawa) propagators D_m and the nucleonic source terms:

$$\phi_B^{(S,I)}(\mathbf{x}) = g_B \int d^3 \mathbf{x}' D_{m_B}(\mathbf{x}, \mathbf{x}') \sum_q \overline{\Psi}_q(\mathbf{x}) \vec{\sigma}^S \vec{\tau}^I \Psi_q(\mathbf{x}')$$
⁽²⁾

where I = 0, 1 denotes iso-scalar and iso-vector meson-nucleon vertices and m_B is the meson rest mass. The (non-relativistic) Hamiltonian density functional is then obtained as

$$\mathcal{H} = \sum_{q} \vec{\nabla} \overline{\Psi}_{q} \frac{\hbar^{2}}{2M_{q}} \vec{\nabla} \Psi_{q} + \frac{1}{2} \sum_{qq',m,S,I} V_{SI}(m) \overline{\Psi}_{q}(x) \vec{\tau}^{I} \Psi_{q}(x) D_{m}(x,x') \overline{\Psi}_{q'}(x) \vec{\tau}^{I} \Psi_{q'}(x')$$
(3)

where $V_{SI}(m) = \frac{\hbar^3 g_B^2}{4\pi m_B^2}$. Expanding this density functional around the expectation value with respect to a nuclear reference state $|A\rangle = |Z, N\rangle$ we obtain the energy density

$$\mathcal{E}(\tau_q, n_q, \kappa_q) = \mathcal{E}_A + \sum_q (h_q n_q + \Delta_q \kappa_q) + \frac{1}{2} \sum_{q, q'} \left(f_{qq'} n_q n_{q'} + w_{qq'} \kappa_q \kappa_{q'} \right)$$
(4)

expressed in terms of kinetic densities (τ_q), number densities (ρ_q), and pairing densities (κ_q) for protons (q = p) and neutrons (q = n), respectively. The first variation leads to the single particle Hamiltonian $h_q = T_q + U_q$ with the self-energy U_q and the pairing gap Δ_q . The second variation results in the residual particle–hole interactions $f_{qq'}$ and the particle–particle interaction $w_{qq'}$, respectively, corresponding to the restoring forces in the respective interaction channels. It should be noted, that both types of residual interactions will depend on the proton and neutron ground state densities $\rho_q(A_q)$. These modifications are given by rearrangement terms, obtained from polarization insertions to propagators and vertices. Normal ordering is assumed for n_q and κ_q , respectively.

3. Pairing and continuum spectroscopy of ¹⁰Li

Away from shell closures pairing effects from particle-particle interactions play a significant role in the spectroscopy, becoming the more efficient the smaller the energy gaps between the unperturbed mean-field levels are. The spectral properties are described [1] in terms of particle- and hole-type states with wave functions $u_{\alpha q}$ and $v_{\alpha q}$, respectively, carrying quantum numbers $\alpha = (n\ell jm)$ and where q = p, n denotes protons and neutrons. The quantity defining the overall dynamics is the single particle mean-field potential U_q . The *u*- and *v*-type states interact in addition through the pairing fields Δ_q . The problem is adequately formulated by the Gorkov equations [1]:

$$\begin{pmatrix} T_q + U_q - 2\lambda_q + e_\alpha & \Delta_q(\vec{r}) \\ -\Delta_q^{\dagger}(\vec{r}) & -(T_q + U_q - e_\alpha) \end{pmatrix} \begin{pmatrix} u_{\alpha q}(\vec{r}) \\ v_{\alpha q}(\vec{r}) \end{pmatrix} = 0$$
(5)

derived in mean-field approximation from Eq. (4).

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