Isospin mixing, Fermi transitions and signatures of nuclear deformation within a mean field approach

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Abstract.
Gamow-Teller and Fermi transitions are considered in a HF+BCS+pnQRPA theoretical framework. We show here how Gamow-Teller strength distributions can be used in a search for signatures of nuclear deformation in neutron-deficient Pb, Hg and Po isotopes, as well as how Fermi transitions allow us to quantify isospin mixing in some even Kr isotopes around $N = Z$.

1 Theoretical framework

Microscopic models describe the structure of the nucleus in terms of the degrees of freedom of its microscopic constituents: the nucleons. Our starting point is a non-relativistic Hamiltonian containing one- and two-body interactions,

$$\hat{H} = \sum_{ij} t_{ij} \hat{a}_i \hat{a}_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_k \hat{a}_l , \quad (1)$$

where $v_{ijkl}$ are the matrix elements of the nucleon-nucleon interaction and the indices $i, j, k$ and $l$ label the single-particle states in some complete orthonormal basis.

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An optimal approximation to the ground state for this Hamiltonian is attained for the wave function \( \Phi \) whose energy expectation value is minimal, that is
\[
\delta \langle \Phi | \hat{H} | \Phi \rangle = 0.
\] (2)

The choice that leads to the Hartree-Fock approximation is a wave function with the form of a single Slater Determinant,
\[
| \Psi \rangle = \prod_{i=1}^{A} a_{i}^{\dagger} |0\rangle,
\] (3)
where the index \( i \) refers to a set of single particle states \( \phi_{i}(\vec{r}) \) to be determined from the variational principle (2).

If we apply the variational principle (2) to the Hamiltonian (1) and consider a trial wave function of the form (3), we get a single particle Hamiltonian, the so called Hartree-Fock Hamiltonian [1]:
\[
h_{kl} = t_{kl} + \sum_{j=1}^{A} \bar{v}_{kjlj} = \epsilon_{k} \delta_{kl}.
\] (4)

By solving these equations, we get the most convenient single particle states. The Hartree-Fock approximation is often called the self-consistent mean-field approximation.

The first feasible Hartree-Fock calculations in nuclei were developed in the seventies by Vautherin and Brink when they included the Skyrme interactions in the formalism [2]. The effective nucleon-nucleon interaction proposed by Skyrme has two parts: a two-body interaction and a three-body interaction,
\[
V = \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk}.
\] (5)

Skyrme proposed a short-range expansion for \( v_{ij} \), that leads to a local potential depending on the velocity; on the other hand, \( v_{ijk} \) is equivalent to a 2-body density dependent interaction. To obtain the Hartree-Fock equations, we have to evaluate the expected value of the Hamiltonian in a Slater determinant, \( E = \langle HF | \hat{H} | HF \rangle \), which is equivalent to computing the spatial integral of a hamiltonian density, \( \int d^{3}r \mathcal{H}(r) \). This hamiltonian density is a functional of certain densities, \( \rho_{q}(r) \), \( \tau_{q}(r) \), \( J_{q}(r) \), and depends also on the Skyrme interaction parameters.

In order to take into account the BCS pairing correlations, we consider a Hamiltonian that contains a pure single-particle part plus a residual interaction acting only on Cooper pairs and whose matrix elements are assumed to be constant:
\[
\hat{H} = \sum_{k} \epsilon_{k} a_{k}^{\dagger} a_{k} - G \sum_{kk' > 0} a_{k}^{\dagger} a_{-k}^{\dagger} a_{-k} a_{k'}. \] (6)
In this case there is an approximate solution based on the BCS ground state,

\[ |BCS⟩ = \prod_{k>0} (u_k + v_k \hat{a}_k^+ \hat{a}_k^-)|0⟩, \tag{7} \]

in which every pair of single-particle levels \((k, -k)\) is occupied with a probability \(v_k^2\) and remains empty with probability \(u_k^2\). Because of this, from now on we will talk about quasiparticles instead of particles. If we consider the variational principle with the constraint that the expected value of the number of particles is conserved,

\[ \delta \langle BCS| \hat{H} - \lambda \hat{N}|BCS⟩ = 0, \tag{8} \]

we can obtain the occupation probabilities as well as the quasiparticle energies. We also get the so-called gap equation,

\[ \Delta = \frac{G}{2} \sum_{k>0} \frac{\Delta}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}, \tag{9} \]

that links the strength of the pairing interaction \(G\) to the gap \(\Delta\), that can be easily computed from the experimental masses.

By means of the QRPA we will study the excited states of the nucleus. In Hartree-Fock models the excited states are the particle-hole excitations, or, in our case, the two-quasiparticle excitations. We consider the variational principle \(\delta \langle \Psi| \hat{H}|\Psi⟩ = 0\) with the Hamiltonian

\[ H = E_0 + \sum_\lambda E_\lambda \alpha_\lambda^+ \alpha_\lambda + \frac{1}{4} \sum_{\mu\lambda'\chi'\chi} V_{\mu\lambda'\chi'} \alpha_\mu^+ \alpha_\lambda^+ \alpha_{\lambda'} \alpha_{\chi'} \tag{10} \]

that admits two-quasiparticle admixtures, the \(\alpha\)’s being the quasiparticle operators. Our new ground state, \(|QRPA⟩\), differs from the Hartree-Fock ground state since it already contains ground state correlations. It is the vacuum of the operator \(\Gamma_\lambda = \sum_{pn} \left[ X^{+\lambda}_{pn} \alpha_n^+ \alpha_p + Y^{+\lambda}_{pn} \alpha_n^+ \alpha_p \right].\)

By using this framework, we will describe charge-exchange processes, as for instance \(\beta\)-decay, on deformed nuclei. It is important to remark that in our formalism the quadrupole deformation is not an input parameter, but it is obtained in a self-consistent way from the mean field. Our single particle states are expanded in eigenstates of an axially symmetric harmonic oscillator, as it is explained in [3].

For the kind of processes we are interested in, the relevant residual interactions are isospin forces giving rise to the allowed Fermi transitions,

\[ V_F(12) = \chi_F (t_1^+ t_2^- + t_1^- t_2^+), \tag{11} \]

and spin-isospin ones leading to allowed Gamow-Teller transitions,

\[ V_{GT}(12) = \chi_{GT} \sigma_1 \cdot \sigma_2 (t_1^+ t_2^- + t_1^- t_2^+). \tag{12} \]
In the QRPA calculation we consider both separable particle-hole and particle-particle interactions. For the particle-hole part we consider a residual interaction, as in [3, 4], and the particle-particle part is a proton-neutron pairing in the $J^\pi = 1^+$ channel.

Now it is easy to compute Fermi and Gamow-Teller strength distributions for each possible final state:

$$B_{F/T}^\pm(\omega) = \sum_f \delta(\omega - \omega_0) |\langle f | T_\pm | 0 \rangle|^2,$$

(13)

$$B_{GT}^\pm(\omega) = \left\{ \sum_{\omega_0} \delta(\omega - \omega_0) |\langle \omega_0 | \sigma_0 t^\pm | 0 \rangle|^2 + 2 \sum_{\omega_1} \delta(\omega - \omega_1) |\langle \omega_1 | \sigma_1 t^\pm | 0 \rangle|^2 \right\}.$$

(14)

2 Gamow-Teller transitions and nuclear deformation

By means of Gamow-Teller strength distributions, we have studied the signatures of nuclear deformation in $\beta$-decay patterns in some neutron-deficient Pb.

![Figure 1. HF energy as a function of the quadrupole deformation $\beta$ for the isotopes $^{184,186,188,190,192,194}$Pb obtained from constrained HF+BCS calculations with the force Sk3 and fixed pairing gap parameters as a function of the quadrupole deformation $\beta$.](image)
Po and Hg isotopes [5]. In fig. 1 it is shown the energy as a function of quadrupole deformation $\beta$ for several lead isotopes. One can observe that in most cases there are three minima close in energy: one corresponding to an oblate shape ($\beta < 0$), another corresponding to a spherical shape ($\beta \approx 0$), and the third one corresponding to a prolate shape ($\beta > 0$).

We have computed the Gamow-Teller strength distributions for each equilibrium deformation and observed that they present different features for each equilibrium deformation. We observe that the strength is distributed differently for the various shapes. The distribution is very fragmented in the oblate case, while it presents a strong single peak at low energy in the prolate case. The spherical case shows a single peak at higher energies. These features can be seen in fig. 2 for the isotope $^{184}\text{Pb}$. These specific signatures prevail against changes in Skyrme forces or pairing treatment and could be used in turn to identify the shape of a $\beta$ decaying nucleus. Currently the GT strength distributions for some of these isotopes are planned to be measured at ISOLDE/CERN [6] in 2007.

Figure 2. Gamow-Teller strength distributions (discrete and folded) in $^{184}\text{Pb}$. The experimental $Q_{EC}$ energy is shown with a dashed vertical line.
3 Fermi transitions and isospin mixing

We have studied Fermi transitions and isospin mixing in some even Kr isotopes around $N = Z$. We know that the self-consistent mean field Hamiltonian breaks the symmetries of the exact Hamiltonian, for instance the total angular momentum is not an exact quantum number for a deformed nucleus. On the other hand, rotational invariance in isospin space is not an exact quantum symmetry of the actual total nuclear Hamiltonian, since the Coulomb force breaks it. We were interested in investigating how important is this isospin breaking and how Coulomb interaction and BCS and QRPA correlations contribute to this mixing. We consider Fermi transitions because for them the effect of isospin mixing is more important.

We have performed QRPA calculations on top of a quasiparticle basis obtained from a self-consistent deformed Hartree-Fock approach with density dependent Skyrme interactions, as it has been already explained in section 1. The Fermi strength distribution can be written as in eq. (13).

Let us assume now that our ground state $|0\rangle$ is an isospin eigenstate. The eigenvalues of the isospin operator acting on this state must be $T_z = (N - Z)/2$ and $T = |T_z|$. Hence, it is clear that:

$$
T_+ |0\rangle = T_+ |T_z\rangle = \sqrt{(Z - N)} |T_z + 1\rangle \quad \text{for } N < Z,
$$

$$
= 0 \quad \text{for } N \geq Z.
$$

$$
T_- |0\rangle = T_- |T_z\rangle = \sqrt{(N - Z)} |T_z - 1\rangle \quad \text{for } N > Z,
$$

$$
= 0 \quad \text{for } N \leq Z.
$$

In other words, by the $\beta^+$ operator there are no accessible states if $N \geq Z$ and by the $\beta^-$ operator there are no accessible states if $Z \geq N$. We will use this “isospin-forbidden” transitions in order to quantify the isospin mixing in our ground state.

The amount of angular momentum mixing [7] in the mean field ground state of axially symmetric deformed nuclei is measured by the expectation value of the squared angular momentum operator perpendicular to the symmetry axis $z$,

$$
\langle J_z^2 \rangle = \langle J^2 \rangle - \langle J_z \rangle^2 = \frac{1}{2} \sum_f |\langle f| J_+ |0\rangle|^2 + |\langle f| J_- |0\rangle|^2.
$$

Similarly, taking the $z$ axis in isospin space in the standard way ($\hat{T}_z = (\hat{N} - \hat{Z})/2$, or $T_z = (N - Z)/2$), we can measure the amount of isospin mixing by the expectation value of $T_z^2 = T_x^2 + T_y^2 = \frac{1}{2} \sum_f \left(|\langle f| T_+ |0\rangle|^2 + |\langle f| T_- |0\rangle|^2\right)$, or better

$$
\langle T_z^2 \rangle_0 = \langle T_z^2 \rangle + \frac{5}{2} \left|\frac{N - Z}{2}\right|.
$$
Isospin mixing, Fermi transitions and signatures of nuclear deformation...

Table 1. Amount of isospin mixing for various approaches in several Kr isotopes.

|       | $\langle T^2 \rangle_0 (\Delta = 0.1 \text{ MeV})$ | $\langle T^2 \rangle_0 (\Delta \sim 1.5 \text{ MeV})$ |
|-------|--------------------------------|--------------------------------|
|       | Coul. | No Coul. | Coul. | No Coul. |
| $^{70}\text{Kr}$ | 0.05  | 0.00    | 0.43  | 0.41    |
| $^{72}\text{Kr}$ | 0.07  | 0.02    | 1.15  | 1.11    |
| $^{74}\text{Kr}$ | 0.03  | 0.00    | 0.50  | 0.44    |
| $^{76}\text{Kr}$ | 0.02  | 0.00    | 0.30  | 0.23    |
| $^{78}\text{Kr}$ | 0.01  | 0.00    | 0.17  | 0.12    |

In the limit in which the ground state is an isospin eigenstate, $T = |T_z| = |(N - Z)/2|$, and $\langle T^2 \rangle_0 = 0$. Therefore $\langle T^2 \rangle_0$ is a good way to measure how important is the isospin mixing.

It can be seen [8] that the value of $\langle T^2 \rangle_0$ is purely due to the correlation terms

$$\langle T^2 \rangle_0 = \langle T^2 \rangle - \frac{|N - Z|}{2} = C_{BCS} + C_{QRPA},$$

and that for $N = Z$ and no Coulomb force $\langle T^2 \rangle_0 \approx 0.$

Taking as a reference the case of a self-consistent mean field calculation, we can see in Table 1 that in the absence of Coulomb interactions (and in the limit

Figure 3. Fermi strength distributions plotted as a function of the excitation energy of the daughter nucleus. The left panels correspond to the case of no Coulomb interaction and pairing gaps approaching zero. The middle panels include also Coulomb interaction. The right panels include both Coulomb interaction and pairing correlations with realistic gaps.
of small pairing correlations) the isospin-forbidden transitions \((\beta^- \text{ in } N \leq Z \text{ and } \beta^+ \text{ in } N \geq Z)\) are negligible. When the isospin-breaking Coulomb interaction is switched on, there is an increase of isospin-forbidden Fermi transitions. Although this increase is small, it is a signature of isospin-breaking. Pairing correlations increase by orders of magnitude the isospin-forbidden Fermi transitions, a fact that is related to the isospin-breaking nature of the quasiparticle mean field, which increases with increasing pairing gaps. On the other hand, the isospin-breaking effects and forbidden Fermi transitions are reduced when RPA correlations are taken into account (see fig. 3).

4 Conclusions

We have studied Gamow-Teller strength distributions in a search for signatures of deformation in neutron-deficient lead isotopes, and Fermi transitions as a measure of isospin mixing in Kr isotopes.

The theoretical framework is a deformed pnQRPA formalism with spin-isospin (GT transitions) or isospin-isospin (F transitions) ph and pp separable residual interactions. The quasiparticle mean field is of Skyrme-HF type including pairing correlations in BCS approximation.

Gamow-Teller strength distributions of neutron-deficient lead isotopes show a strong dependence on nuclear deformation, which remains against changes of the Skyrme and pairing forces. We conclude that \(\beta^-\)-decay of these isotopes could be a useful tool to look for fingerprints of nuclear deformation.

We have studied isospin mixing properties in several Kr isotopes around \(N = Z\) and analyzed their Fermi transitions at various levels of approximation. We have considered self-consistent deformed Skyrme HF mean fields with and without Coulomb and pairing interactions. Then, we take into account isospin-dependent residual interactions and consider QRPA correlated ground states. We have studied the effect on the Fermi strength distributions of isospin-breaking interactions (Coulomb force and pairing), as well as the effect of QRPA correlations including Fermi type residual interactions, whose particle-hole strengths are consistently fixed with the Skyrme force. Starting from strict Hartree-Fock approach without Coulomb, it is shown that the isospin breaking is negligible, on the order of a few per thousand for \((N - Z) = 6\), increasing to a few percent with Coulomb. Pairing correlations induce rather large isospin mixing and Fermi transitions of the forbidden type \((\beta^- \text{ for } N \leq Z, \text{ and } \beta^+ \text{ for } N \geq Z)\). The enhancement produced by BCS correlations is compensated to a large extent by QRPA correlations induced by isospin-conserving residual interactions that tend to restore isospin symmetry.

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