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An algorithm of constructing potential energy surfaces for nuclear particle-hole excited configurations*

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We discuss and illustrate a computer-designed algorithm allowing to construct the nuclear potential energy surfaces generated by a mean field Hamiltonian $H(\alpha)$ as functions of the ensemble of nuclear deformation variables α for multi-particle multi-hole excited configurations. The algorithm in question serves to eliminating the undesired effect of the so-called avoided crossing mechanism, a consequence of the well known property referred to as Landau-Zener non-crossing rule.

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1. Introduction

In this article we discuss an algorithm of calculating nuclear potential energy surfaces for the multi-particle multi-hole excitations using the mean-field approach. The underlying problem is related with the mechanism known in many applications of quantum mechanics and in particular in quantum chemistry under the name of *avoided crossing*-, sometimes: non-crossing or intended crossing mechanisms, also: Landau-Zener non-crossing rule, cf. e.g. ref. [1]. More precisely: Consider eigenvalues of an Hermitian matrix depending on n continuous, real parameters. The eigenvalues can be treated as functions of these parameters and as it turns out, in general they cannot become equal for any choice of parameters in the considered n -dimensional space. In the present context, the Hermitian matrix in question will be identified with the nuclear mean-field Hamiltonian depending on n real deformation parameters.

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In order to describe the particle-hole excitation energies in the deformation space considered, special care needs to be taken of the single-particle level crossings – which are numerous, when the evolution of the nuclear shape in the deformation spaces is studied. More precisely, if Hamiltonian of the studied system is symmetric under some symmetry group, then the description of the level-crossings in the single particle spectra usually follows one of the two possible scenarios.

According to the first of those scenarios, when two given single-particle states belong to the same irreducible representation of the symmetry group, the corresponding energies may approach each other when the deformation changes, but they do not cross as the result of the just mentioned Landau-Zener non-crossing rule. Thus the levels which at the increasing deformation approach each other, and next evolve as if “repelling each other without touching”, cf. full lines in the schematic illustration in Fig. 1, right panel, representing the situation referred to as *non-crossing* or *pseudo-crossing*.

In contrast, the states belonging to the different irreducible representations “can simply cross” (Landau-Zener rule does not apply), as illustrated by two straight dashed lines in Fig. 1, left panel.

Let us emphasise that in nuclear structure physics the same rules apply also to another case of strong interest, *viz.* description of nuclear rotation in terms of the cranking approximation, where the role of the deformation parameters is played by the rotation (cranking) frequencies, $\{\omega_x, \omega_y, \omega_z\}$. In this particular case we may rather straightforwardly learn about the nuclear system preferences as far as the way of transiting through the crossing zones is concerned: Does the system evolve through the crossing by following always the lowest level (full line in Fig. 1, right) – or – does it “jump” by continuing the evolution along the prolongation of the lower level as if crossing never existed? To answer this question it will be instructive to recall that the derivative of the single-particle level with respect to the cranking frequency gives, up to the sign, the single particle angular momentum alignment, here denoted j_ν^ω . Indeed, consider rotation about the \mathcal{O}_x -cranking axis. Omitting index x for simplicity we have

$$j_\nu^\omega = -\frac{de_\nu^\omega}{d\omega} \rightarrow I^\omega = \sum_{\nu \in \text{occ.}} j_\nu^\omega \rightarrow \mathcal{J}^\omega \equiv \frac{I^\omega}{\omega}, \quad (1)$$

where I^ω and \mathcal{J}^ω are, respectively, the aligned angular momentum and kinematical moment of inertia, both easily accessible *via* experiment. Comparison with numerous experimental results shows that the nuclear system in the great majority of the known cases follows the scenario of a direct jump ‘as if the crossing did not exist’.

Similar can be said about the energy dependence on deformation.

2. Description of single-particle level crossing

In the considered nuclear context the numerical algorithms begin with solving the Schrödinger equation usually via diagonalisation of the nuclear mean-field Hamiltonian employing the harmonic oscillator basis. The solutions of the mean-field problem are the single-nucleonic orbitals $\{e_\nu, \psi_\nu\}$ and the first problem which arises at this stage is the choice of labelling (more generally: identification) of the corresponding solutions. A possible way out is to apply the single-particle so-called Nilsson labelling, ref. [2]. In this case, the single particle levels are labeled with a set of quantum numbers characterising the harmonic oscillator basis-state leading in the expansion. For example the asymptotic quantum numbers such as the main harmonic oscillator shell N , the number of quanta in the z -direction, n_z , the projection of the orbital angular momentum on the symmetry axis, Λ , and the corresponding projection of the total angular momentum, Ω , define the set denoted $[Nn_z\Lambda]\Omega$ which can be used as a label.

In the case of the Nilsson model the above scheme turned out to be very useful since the dominating harmonic-oscillator basis-states appeared in the expansion of the solutions with the very large amplitude (or probability). This characteristic domination gave a strong justification for the use of this labelling. As it turns out, the levels which have the same (very similar) slope before and after the crossing keep the same Nilsson labelling. This information could be conveniently used to treat the avoided level crossings within numerical algorithms.

In the case of more realistic potentials, *e.g.*, ‘Woods-Saxon universal’ model family, ref. [3], the scheme described above is a much less evident choice since the leading wave functions may appear in the expansion of the solutions with the probabilities of the order of 10-to-15% and as it turns out several harmonic oscillator wave functions may appear with the comparable amplitudes. As one of the implications, more than one single particle solution may appear with the same label. Despite the above caution it is still common in the literature to use this labelling of the single particle orbitals. Thus the quantum numbers corresponding to the basis state with the largest amplitude, even if the next important one differs from the preceding one in terms of the probability amplitudes only insignificantly, are usually used as labels.

As we shall see, in the case of the realistic Hamiltonians (potentials) the discussed labels of states are changing along with the deformation parameters and are in the present context not very useful. Therefore we intend to employ the information about the whole intrinsic structure of the orbitals, which remains robust when deformation varies. These properties will be employed and discussed in the following.

3. The case of a two-level model

Let us first consider a simplified-model real-Hamiltonian H having only two eigenstates. The matrix representation of H within a basis say, ϕ_1 and ϕ_2 , can be given as:

$$H_{k,\ell} \rightarrow \begin{bmatrix} -e & v \\ v & e \end{bmatrix}. \quad (2)$$

Figure 1 can be seen as a schematic illustration of two alternative situations:

- Non-mixed states (left panel): interaction $v = 0$;
- Mixed states (right panel): interaction $v \neq 0$.

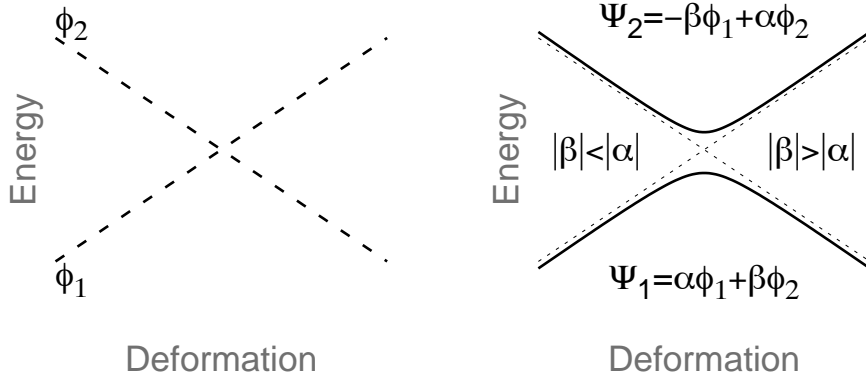


Fig. 1. Schematic illustration of the two discussed variants of the level crossing. Left: No mixing and no repulsion of levels, levels cross. Right, full lines: Mixing, the levels repel each other.

The wave functions Ψ_i for $i = 1, 2$ can be represented as follows. For the non-mixed states ($v = 0$) one may select $\Psi_1 = \phi_1$ and $\Psi_2 = \phi_2$, whereas for the case of $v \neq 0$ one has

$$\Psi_1 = +\alpha\phi_1 + \beta\phi_2, \quad (3)$$

$$\Psi_2 = -\beta\phi_1 + \alpha\phi_2, \quad (4)$$

where

$$|\alpha|^2 + |\beta|^2 = 1. \quad (5)$$

At the crossing point, the amplitudes are equal, *i.e.*, $|\alpha| = |\beta| = 1/\sqrt{2}$. Traversing the crossing point leads to the exchange of the structure of Ψ_1

and Ψ_2 . For instance, one has for Ψ_1 on the left hand side of the crossing point $|\alpha| > |\beta|$ whereas on the right hand side of the crossing point $|\beta| > |\alpha|$. The commonly used identification of the structure of states according to the labels attached to Ψ_1 and Ψ_2 becomes misleading. To respect the structure content of the wave functions, the label “1” of the *lower* level before the pseudo-crossing should be used to label the *upper* level after the pseudo-crossing point, with the similar manipulation for the other pair of levels.

The problem posed is the following: How to construct an automatic, computer programmable algorithm, which in the realistic Hamiltonian case connects the levels of the same structure before the crossing and after the crossing, rather than connecting the levels according to the energy order: “the first level connected always with the first level, “the second level connected always with the second level”, etc.

4. Identification of levels before avoided-crossing removal

Let us consider two successive deformation points, the one to the left of the crossing point, labelled with the letter L and another one, to the right of the crossing point, labelled with the letter R (see Fig. 2). Both points are selected in such a way, that in the present context L and R can be considered “sufficiently close” to each other.

We say that a single particle state ${}_R\langle k|$ at R is of a similar structure compared to the state $|m\rangle_L$ at L , if and only if the absolute value of the scalar product of corresponding eigenvectors at L and R is close to 1, *i.e.*,

$$|{}_L\langle k|m\rangle_R| \approx 1. \quad (6)$$

Otherwise they are considered being of dissimilar structure and satisfy $|{}_L\langle k|m\rangle_R| \approx 0$. The above property can be considered as an extension of the notion of the orthonormality of eigenvectors for some neighbouring points L and R .

The above scheme is directly applicable to the realistic nuclear mean-field Hamiltonians, e.g., for the case of the Woods-Saxon potential:

- After calculating all the eigenvectors of interest, $\{{}_L\langle k|\}$ and $\{|m\rangle_R\}$, at deformation points L and R , respectively, one calculates the corresponding overlaps. These overlaps are used to identify the *pairs* of levels $\{k, m\}$ for which the scalar product $|{}_L\langle k|m\rangle_R| \approx 1$.
- For the appropriately chosen deformation-distance between L and R , all but one pair of considered vectors are approximately orthogonal. This information completes the necessary criterion for connecting the levels which pass through the avoided crossing zones.

One may formulate this property alternatively as follows. Inspired by illustration in Fig. 2, we consider two states arbitrarily called *lower*, $\langle k_\ell |$, and *upper*, $\langle k_u |$, both at L and similarly *lower*, $|m_\ell\rangle$, and *upper*, $|m_u\rangle$, both at R . One expects two following situations:

- If there is no crossing the following approximate relations hold

$$|\langle k_\ell | m_\ell \rangle| \sim 1, \quad (7)$$

$$|\langle k_u | m_u \rangle| \sim 1, \quad (8)$$

$$|\langle k_\ell | m_u \rangle| \sim 0, \quad (9)$$

$$|\langle k_u | m_\ell \rangle| \sim 0. \quad (10)$$

- In the case of the crossing of levels k and m the following relations are approximately valid:

$$|\langle k_\ell | m_\ell \rangle| \sim 0, \quad (11)$$

$$|\langle k_u | m_u \rangle| \sim 0, \quad (12)$$

$$|\langle k_\ell | m_u \rangle| \sim 1, \quad (13)$$

$$|\langle k_u | m_\ell \rangle| \sim 1. \quad (14)$$

The above system of conditions allows to identify the levels which go straight from L to R without crossing and thus for constructing of the particle-hole excitation energies and the corresponding total potential energy surfaces.

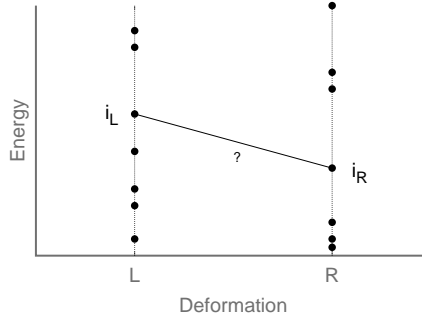


Fig. 2. Schematic illustration. Full dots represent energies of single particle states at the selected deformation points labelled L and R , which have to be joined according to some identification rule. In the present article we select the size of the absolute value of the scalar product of the corresponding eigenstates.

5. An illustrative example

In this article we employ the nuclear mean-field approach with the standard phenomenological “universal” Woods-Saxon Hamiltonian of refs. [3]. Figure 3 shows the spectrum of the single particle proton levels in ^{86}Kr . The spectrum was generated using Woods-Saxon potential.

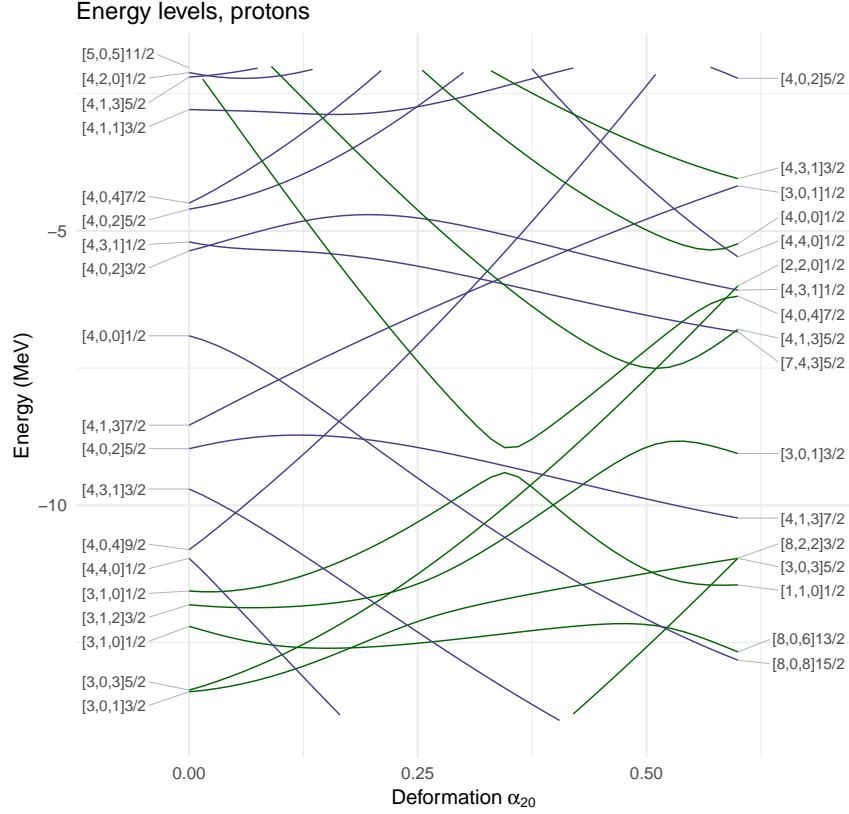


Fig. 3. Proton single particle energy levels obtained using the deformed Woods-Saxon potential (with the so-called “universal parameters”) for $^{86}_{36}\text{Kr}_{50}$. We use the asymptotic type Nilsson labels $[Nn_z|\Lambda]\Omega$.

In the following Figures we illustrate the potential energies of the 2-quasiparticle excited configurations for neutrons and protons obtained by employing the above algorithm. As expected, the minima of excited states generally differ, sometimes considerably, as compared to the minimum of the ground state of the nucleus.

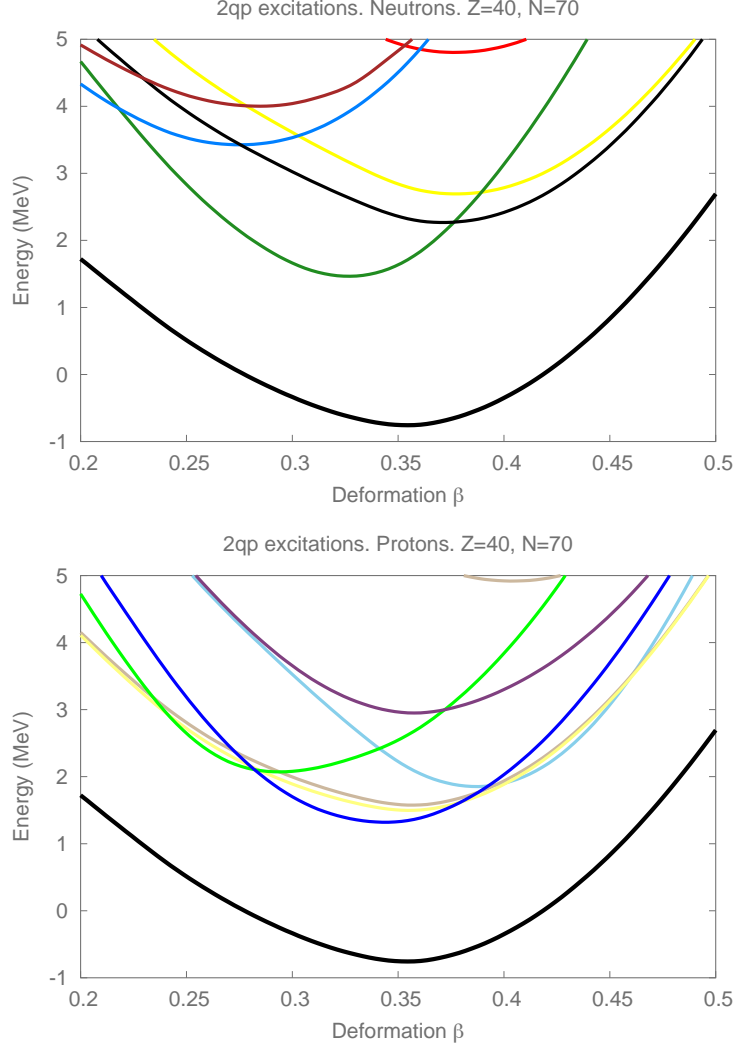


Fig. 4. Lowest 2-quasi-particles neutron energy levels (upper part of the Figure) and proton ones (lower part of the Figure) in Woods-Saxon potential for $^{110}_{70}\text{Zr}_{40}$. The black curve represents the energy of the ground state of the nucleus.

6. Conclusions

In the present note we discuss a proposition of an automatic algorithm serving to connect the nuclear mean-field single-particle energy levels through the avoided-crossing zones by employing the criteria of structural similitude of the orbitals before and after the crossing zone. The algorithm

uses the criterion of the maximum overlap of eigenfunctions associated with the connected energy levels. With the help of this algorithm potential energy surfaces corresponding to multi-particle multi-hole excited configurations as well as many-quasiparticle-excitations treated as functions of the deformation can be constructed.

The same algorithm can be straightforwardly used for calculating the nuclear energies of the rotational states treated as functions of the cranking frequencies before conveniently transforming them into energy vs.-spin representation for easier comparison with experiment.

7. Acknowledgments

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 This approach is being used without modifications by many authors also today.