Self-consistent constrained HFB in odd-A nuclei†

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All existing constrained Hartree-Fock-Bogoliubov (CHFB) calculations neglect the Fock or the exchange terms. Here, the constraint conditions are applicable to the proton number Z, neutron number N, and the angular momentum along the chosen x-axis $\langle I_x\rangle = \sqrt{I(I+1)}$. The numerical calculations start from the spherical single-particle basis and include the residual quadrupole-quadrupole (Q-Q), monopole-pairing (MP), and quadruple-pairing (QP) interactions.[1] In the approximation without the exchange terms, only the terms Y^2_0 and $Y^2_2 + Y^2_{-2}$ in the Q-Q interaction are considered but the terms $Y^2_1 \pm Y^2_{-1}$ and $Y^2_2 - Y^2_{-2}$ are not. We have developed the code to include all exchange terms in the residual interactions. The exchange terms of Q-Q contribute to the self-energy Γ and the gap Δ, and those of MP and QP to Γ. Then, the constraint on angular momentum $\langle I_x\rangle$ becomes $\sqrt{I(I+1) - \langle I^2_z\rangle}$. We chose the signature invariant base that reduces the diagonalization space to half[2] because the total Hamiltonian with three constraints H' is invariant under the operator $R_x = \exp(-i\pi I_x)$. All input matrix elements are rewritten in this base and the spherical single-particle operator in this base C_k is transformed to quasiparticle operators $\alpha^\dagger_i = \sum_{k>0}(C^\dagger_k A_{ki} + C_{\hat{k}} B_{ki})$ and $\alpha^\dagger_{\hat{i}} = \sum_{k>0}(C^\dagger_{\hat{k}} \hat{A}_{ki} + C_k \hat{B}_{ki})$, where the notation $\hat{k}$ is the time reversal of k. Then, the CHFB equation becomes:

$$\begin{pmatrix} h^1 - \omega j_x & \Delta^T \\ \Delta^* & -h^{2*} - \omega j_x \end{pmatrix} \begin{pmatrix} \hat{B}^* & A \\ \hat{A}^* & B \end{pmatrix} = \begin{pmatrix} \hat{B}^* & A \\ \hat{A}^* & B \end{pmatrix} \begin{pmatrix} -\hat{\Lambda} & 0 \\ 0 & \Lambda \end{pmatrix}, \quad (1)$$

where h^1 (h^2) includes the spherical single-particle energy and self-energy Γ and ω is the Lagrange multiplier for $I_x = \sum_{k,l>0}(j_x)_{k,l}(C^\dagger_k\ C_l - C^\dagger_{\hat{k}} C_{\hat{l}})$. When there is no ωj_x, *i.e.*, without constraint on $\langle I_x\rangle$, h^2, $\hat{\Lambda}$, $\hat{A}$, and $\hat{B}$ are reduced to h^1, Λ, A, and B, respectively. The iteration procedure in the numerical analysis is based on the gradient method.[3]

Figure 1 compares I versus transition energy $\Delta E = E(I) - E(I-2)$. The parameters are the same spherical single-particle energy as listed in Table 1 in Ref. 1). The strength of MP is $G^{(0)}_{\pi+\pi+} = G^{(0)}_{\pi-\pi-} = G^{(0)}_{\pi+\pi-} = -0.22$ MeV and $G^{(0)}_{\nu+\nu+} = G^{(0)}_{\nu-\nu-} = G^{(0)}_{\nu+\nu-} = -0.23$ MeV. The strength of QP is 10% of MP, expressed in terms of MeV/b^4 and the strength of QQ is $\chi_{\pi\pi} = -0.030$ MeV/b^4, $\chi_{\nu\nu} = -0.032$ MeV/b^4, and $\chi_{\pi\nu} = -0.100$ MeV/b^4 with an oscillator length b. These numerical results are consistent with the experimental data except for the $I = 15/2^-$ state. The constraint on the proton number Z is effective but the value of Z for + and − parity states is mixed owing to $G^{(0)}_{\pi+\pi-}$. For example, $Z_+ = 13.58$ and $Z_- = 17.42$ at $I = 15/2^-$, while $Z_+ = 13.99$ and $Z_- = 17.01$ at $I = 55/2^-$, where $Z = Z_+ + Z_-$ is the proton number outside the magic number 28. For better results, another constraint on $Z-$ should be included or the MP and QP interactions between the + and − parity states should be dropped. This calculation is preliminary and there is room for finding better parameter sets.

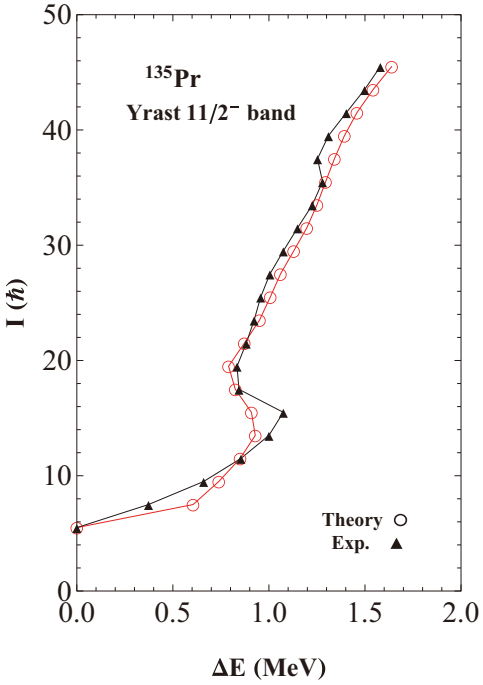

Fig. 1. Backbending plot for I as a function of energy difference $\Delta E = E(I) - E(I-2)$. Experimental data is taken from Ref. 4).

† Condensed from the talk in Int. Symp. on "Simplicity, Symmetry and Beauty," Sept. 26–28, Shanghai (2018)
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