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A New Iterative Approach for the Exact Solution of the Standard Pairing Model

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Abstract: A new iterative approach for solving the standard pairing problem is established based on polynomial approach. It provides an efficient way to derive the particle-number conserved pairing wave functions for both spherical and deformed systems, especially for large-size systems. The method reduces the complexity of solving a system for k-pairs polynomial equations into a system for one-pair polynomial equation, which can be efficiently implemented by the Newton-Raphson algorithm with a Monte Carlo sampling procedure for providing the initial guesses step by step. The present algorithm can also be used to solve a large class of Gaudin type quantum many-body problems as a more than 100 orbitals and 50 pairs system such as super-heavy nuclei and nuclear fission.

Key words: standard pairing problem, iterative approach, super-heavy nuclei, nuclear fission

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1 Introduction

Nuclear pairing correlation, similar to the pairing correlation in the Bardeen-Cooper-Schrieffer (BCS) theory of superconductors, is a key ingredient from the residual interactions of the nuclear shell model in elucidating properties of the ground states and low-energy spectra of nuclei, such as binding energies, odd-even effects, single-particle occupancies, excitation spectra, electromagnetic transition rates, beta-decay probabilities, and so on[1–6]. The simple BCS approximation and the generalized Hartree-Fock-Bogoliubov (HFB) theory are successful in describing the pairing properties of open-shell nuclei. However, as an approximate theory, both the BCS and the more refined HFB methods suffer from serious drawbacks in nuclei due to the fact that the number of valence nucleons under the influence of the pairing force is too few to be treated by such particle-number non-conserved (quasi-particle) approximations[7–9]. Alternatively, shell model calculations provide successful descriptions but face a combinatorial growth of model space sizes, and hence, for heavy nuclei, truncation schemes are normally needed and applicability is often limited by existing computer resources. The Projected Shell Model (PSM) provides a way to overcome this difficulty[10]. By using the PSM scheme, it is shown that the projected BCS vacuum for a well-deformed system is very close to the $SU(3)$ dynamical symmetry limit of an S-D pair fermion system[11]. An exact solution of the standard pairing problem was first obtained by Richardson and is now referred to as the Richardson-Gaudin method[12–13]. It has been observed recently[14] that solutions of the standard pairing model can be obtained from zeros of the associated extended Heine-Stieltjes polynomials, which makes it feasible to apply the model with many valence nucleon pairs over a large number of single-particle levels. Furthermore, by using the extended Heine-Stieltjes polynomials, the Nilsson mean-field plus standard pairing model is applied to describe the ground state phase transition in Nd, Sm, and Gd isotopes, the analysis provides a microscopic picture that the ground state phase transitional behaviors may be driven by the competition between the Nilsson mean-field and the pairing interaction based on the present model[15]. In addition, a recent study[16] provides a refined method to solve the nonlinear Richardson equation for both deformed and nearly spherical nuclei based on the polynomial approaches shown in Refs. [17–18].

In this paper, we try to provide a new iterative approach to guess the initial values step by step, which based on the fast Newton-Raphson algorithm with a Monte Carlo sampling procedure. The goal of this paper is to provide a flexible and practical approach which can be used to solve a large class of Gaudin type

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quantum many-body problems such as super-heavy nuclei and nuclear fission.

2 The mean-field plus standard pairing model and its exact solution

The Hamiltonian of the standard pairing model is given by

$$\hat{H}=\sum_j \epsilon_j \hat{n}_j - G\sum_{jj'} S_j^+ S_{j'}^-, \tag{1}$$

where the sums run over given j-levels of total number n, $G>0$ is the overall pairing strength, ϵ_j are non-degenerate single-particle energies, $\hat{n}_j=\sum_m a_{jm}^\dagger a_{jm}$ is the number operator for valence particles in the j-th level, and $S_j^+=\sum_m(-)^{j-m}a_{jm}^\dagger a_{j\,-m}^\dagger$ $(S_j^-=(S_j^+)^\dagger)$ are pair creation (annihilation) operators. The formalism is first presented for an even number of particles that are all paired (seniority-zero case), while the generalization to an additional odd unpaired particle is discussed in relation to the pairing eigen-energies. For deformed system (doubly-degenerate orbitals as Nilsson levels), $n_i=a_{i\uparrow}^\dagger a_{i\uparrow}+a_{i\downarrow}^\dagger a_{i\downarrow}$ is the fermion number operator for the i-th doubly-degenerate orbitals, and $S_i^+=a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger$ $[S_i^-=(S_i^+)^\dagger=a_{i\downarrow}a_{i\uparrow}]$ is pair creation [annihilation] operator, The up and down arrows in these expressions refer to time-reversed states.

According to the Richardson-Gaudin method, k-pair eigenstates of Eq. (1) can be written as

$$|k;x\rangle=S^+(x_1)S^+(x_2)\cdots S^+(x_k)|0\rangle, \tag{2}$$

where $|0\rangle$ is the pairing vacuum state satisfying $S_j^-|0\rangle=0$ for all j, x_i $(i=1,2,\cdots,k)$ are spectral parameters to be determined. It can then be verified by using the corresponding eigen-equation that Eq. (2) is the eigenstates of Eq. (1) only when the spectral parameters x_i satisfy the following set of Bethe ansatz equations:

$$1-2G\sum_j\frac{\rho_j}{x_i-2\epsilon_j}-2G\sum_{\substack{i'=1\\(\neq i)}}^{k}\frac{1}{x_i-x_{i'}}=0, \tag{3}$$

where the first sum runs over all j-levels and $\rho_j=-\Omega_j/2$ with $\Omega_j=j+1/2$. For each $x^{(\xi)}$ solution, the corresponding eigen-energy is given by $E_k^{(\xi)}=\sum_{i=1}^k x_i^{(\xi)}$.

According to the polynomial approach in Refs. [16–18] one can find solutions of Eq. (3) by solving the second-order Fuchsian equation Ref. [14]:

$$A(x)P''(x)+B(x)P'(x)-C(P,x)P(x)=0, \tag{4}$$

where $A(x)=\prod_{j=1}^n(x-2\varepsilon_j)$, $B(x)=\left(\frac{1}{G}+\sum_j\frac{\Omega_j}{x-2\varepsilon_j}\right)$ and $C(P,x)=\sum_{j=1}^n\frac{\Omega_j}{x-2\varepsilon_j}\left(\frac{P'(2\varepsilon_j)}{P(2\varepsilon_j)}\right)A(x)$. The polynomials $P(x)$ with zeros corresponding to the solutions of Eq. (3), which defined as

$$P(x)=\prod_{i=1}^k(x-x_i)=\sum_j^k a_j x^j, \tag{5}$$

where k is the number of pairs and a are the expansion coefficients to be determined and a_j become the unknown variables instead of the Richardson variables x_i. Furthermore, if we set $a_k=1$ in $P(x)$, the coefficient a_{k-1} becomes equal to the negative sum of the $P(x)$ zeros, $a_{k-1}=-\sum_i^k x_i=-E_k$.

Particulary, If the value of x approaches twice the single-particle energy of a given orbital j_δ, *i.e.*, $x=2\varepsilon_\delta$, one has

$$\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)^2+(1-\Omega_\delta)\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)'-\frac{1}{G}\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)$$
$$=\sum_{j\neq\delta}\frac{\Omega_j}{2\varepsilon_\delta-2\varepsilon_j}\left[\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)-\left(\frac{P'(2\varepsilon_j)}{P(2\varepsilon_j)}\right)\right]. \tag{6}$$

For doubly degenerate case, above equation set reduces to a much simpler one as

$$\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)^2-\frac{1}{G}\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)-$$
$$\sum_{j\neq\delta}\frac{\left[\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)-\left(\frac{P'(2\varepsilon_j)}{P(2\varepsilon_j)}\right)\right]}{2\varepsilon_\delta-2\varepsilon_j}=0. \tag{7}$$

3 Iterative approach

The most time-consuming part of the numerical algorithm is related to finding the roots of k coupled polynomials in the unknown $a_{0,\ldots,k-1}$ coefficients in Eq. (6). The Newton-Raphson algorithm (NR), which is an extremely fast algorithm given an initial guess $\{a_0^0,\ldots,a_{k-1}^0\}$. The grid of initial guesses is selected by using a Monte Carlo sampling within the boundaries of the $\{a\}$ coefficients derived from physical conditions. The problems with the original method based on the NR algorithm in Refs. [16–17] relate to detecting a singular Jacobian matrix, which is irrelevant when a Monte Carlo sampling is used, as it already perturbs the initial guesses by choosing random numbers. So if only a few initial guesses $\{a\}$ input at the same time, the convergence speed of the NR algorithm is really fast, while, when more initial guesses $\{a\}$ are considered, the detecting polynomial $P^0(x)$ in Eq. (5) will be far from the real form of $P(x)$ that may lead to more consuming time or even return a non-convergence solution.

The new iterative approach to guess the initial values of $a_{0,\ldots,k-1}$ in Eq. (6) is also based on the NR algorithm with a Monte Carlo sampling procedure. For a system with n orbitals and k pairs $(n\geqslant k)$,

firstly, we guess the initial values of $a_{0,\ldots,k-1}$ in Eq. (6) from champions systems with a small number of pairs, k=1 and the number of orbitals n=1, by using the NR algorithm find the real form of $P_1(x) = (a_0 + x)$, and then according to $P_1(x)$ as well as the physical conditions guess the initial values $\{a_0^0, a_1^0\}$ from $P_2^0(x) = P_1(x) \times (x - 2\epsilon_j + r)$ for k=2, n=2 case, r is a random number from Monte Carlo sampling box. In addition, substitute $P_2^0(x)$ in Eq. (5), similarly, the NR algorithm employed to find the real form of $P_2(x) = (a_0 + a_1 x + x^2)$. Following this process, iterate k times to find the $P_k(x)$ for k pairs and $n = k$ orbitals system. Due to the number of $\{a_k\}$ coefficients interrelated to the number of orbitals n, in the next loop, we set $P_k(x)$ which obtained above as the initial values to guess solutions from the $n = k+1$ orbitals to n orbitals, the corresponding step is increasing one orbital each time. Finally, the exact pairing solutions for the n orbitals and k pairs system are calculated following all those steps. The limitation of the new iterative approach is that the Eq. (5) claims $n \geqslant k$, so for the spherical system with $n < k$ is not within the scope of application. While for the deformed system as well as the spherical system with $n \geqslant k$, by using the new iterative approach, the k-dimensional Monte Carlo sampling procedure is reduced to the one-dimensional Monte Carlo sampling procedure which significantly improved the computational efficiency. This makes the exact pairing solutions feasible even when more energy levels or super-heavy nuclei are considered. The largest system we handled at the current calculation is with 50 pairs and more than 100 orbitals, the calculation efficiency is for k=10, k=20, k=30 and n=100 roughly takes 50 s, 1.2 min and 2.5 min on a usual desktop with Intel Core i7-2600k 3.40 GHz processor, that is practically enough for all nuclear pairing problems. Especially, compared to the original method in Refs. [16–17], lost of precision or failure to detect a zero typically result in missing solutions or providing solutions that are far from convergence are avoided for a large number of solution sets, that is reasonable for most realistic applications in nuclear physics. Furthermore, the new iterative approach can be easily extended and applied to solve a large class of Gaudin-type quantum many-body problems.

4 Discussion

4.1 Numerical analysis

To demonstrate the computational complexity of the iterative approach, we consider the examples of $n = 1,\ldots,50$ energy orbitals, the numbers of pairs from k=1,…,25 pairs. For all applications, the single-particle energies used in Eq. (6) are equal spacing $\epsilon_i = i/10$ MeV, $i = 0,1,\ldots,n$ and the pairing strength G=0.001, 0.008, 0.025 and 0.032 MeV. Fig. 1 and Fig. 2 show the ground-state energy of the Hamiltonian Eq. (1) as function of k as well as n for both the doubly-degenerate with $\Omega_i = 1$ ($j = 1/2$) and high degenerate with $\Omega_i = 1,\ldots,k$ ($j = 1/2,\ldots,k/2$) cases. As show in Fig. 1 and Fig. 2, the advantage of the iterative approach is obvious that it avoid the non-solutions problem in Ref. [17] and the numerical unstable fluctuation in Ref. [16], the computational efficiency has been significantly improved. Those results indicate the new iterative approach is more feasible and reliable in solving the standard pairing model and easily apply to the large nuclear systems even for open shell calculations. Especially compared to the doubly-degenerate

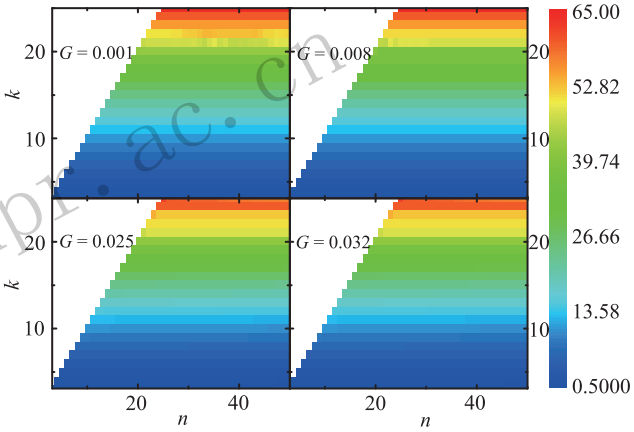

Fig. 1 (color online) The ground-state energy (in MeV) as a function of the orbital number n as well as the number of pairs k=10 for a doubly-degenerate system with $\Omega_i = 1$ ($j = 1/2$) and the pairing strength G=0.001, 0.008, 0.025 and 0.032 MeV under the present model.

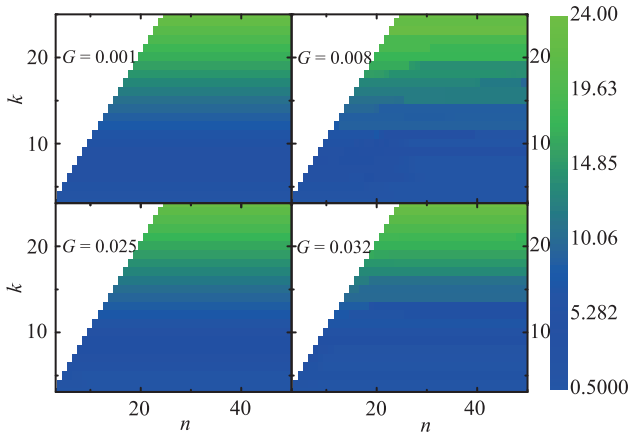

Fig. 2 (color online) The ground-state energy (in MeV) as a function of the orbital number n as well as the number of pairs $k = 10$ for a high degenerate system with $\Omega_i = 1,\ldots,k$ ($j = 1/2,\ldots,k/2$) and the pairing strength G=0.001, 0.008, 0.025 and 0.032 MeV under the present model.

systems(Fig. 1), systems with high degeneracies will be more challenging to solve. While for the high degeneracies systems, the iterative approach demonstrates the same powerful processing (Fig. 1). Therefore, the new iterative approach indeed can be straightforwardly applied for both the doubly-degenerate systems and degeneracies systems with large model spaces.

4.2 Role of the pairing interaction

Larger valence spaces that are necessary for good descriptions of heavier systems which are typically very difficult to be solved directly by employing the original method. To gain the insight into the possible role of the valence spaces as well as the pairing interaction under the present model, the variation of ground-state energy as a function of the orbital number n and the pairing interaction strength G is studied based on the new iterative approach. Fig. 3 displays ground-state energy obtained from the model space with $n=1,\ldots,100$ orbitals and $k=10$ pairs, the single-particle energies are equal spacing $\epsilon_i = i/10$ MeV, $i = 0,1,\ldots,n$ and degeneracy $\Omega_i = 1$ $(j = 1/2)$. It is clearly shown that ground-state energy has an obvious change by varying the pairing interaction strength from G=0 to G=0.05 MeV and the orbital number from n=10 to n=100. Particularly, the lowest energy E=6.8 MeV appears in the point of n=100 and G=0.05 MeV, which naturally demonstrates that as an attraction, the contribution of the pairing interaction is making the total energy of the system become lower. Furthermore, for a given number of pairs, when more orbitals are taken into account, the effect of the pairing interaction is enhanced under the present model and the pairing interaction is inversely proportional to the valence spaces for the given values of ground-state energy that is clearly described by the behavior of the iso-energy curve shown in Fig. 3 As a short-range interaction, the effect of the pairing interaction will be greatly weakened after the half-filled cases (see Fig. 3 with $n>20$).

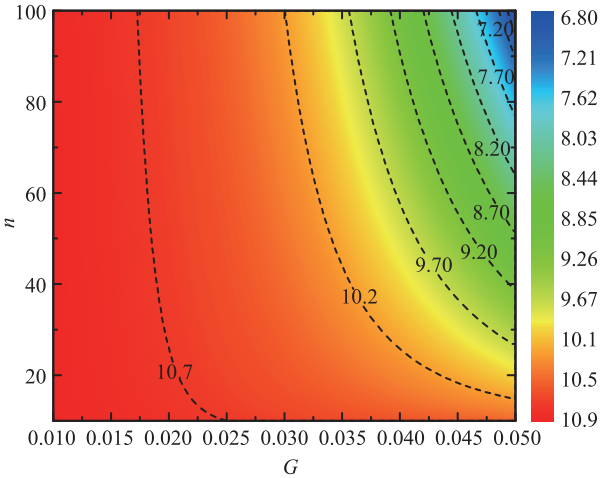

Fig. 3 (color online) The ground-state energy (in MeV) for a doubly-degenerate equally spaced model with the number of pairs k=10, as a function of the orbital number n as well as the pairing interaction strength G.

4.3 The odd-even mass differences of Sm isotopes

The odd-even mass differences of Sm isotopes will be fitted by using the iterative approach of standard pairing model as examples to explore the feasibility in large nuclear systems. we consider a realistic example with a focus on Sm isotopes that adopts single-particle energies from the Woods-Saxon potential in which the deformation parameters β_2 and β_4 values extracted from Ref. [19]. As an approximation, two valence model space consisting of the sixth and seventh major shell with 51 single-particle orbits for valence neutrons will be considered and the proton pairs excitation will be ignored. The odd-even mass difference is defined as $\Delta_c^{(3)} \equiv \frac{1}{2}(E_B(Z,N)-2E_B(Z,N-1)+E_B(Z,N+1))$[20], where $E_B(Z,N)$ is the binding energy, Z and N are proton and neutron number, respectively. For the odd-A systems, the levels blocked by the odd particle are obtained from the lowest theoretical energy.

For pairing strength G=0.06 MeV, the odd-even mass differences obtained using the present approach are found to reproduce the experimental data remarkably well (Fig. 4). The consistency between the experimental and the theoretical results shown in Fig. 4 indicates that the present model describes the ground state quantities of these nuclei rather well, the iterative approach can be straightforwardly applied for heavy nuclear systems and large model spaces, super-heavy nuclei and unclear fission are a possible to be handled.

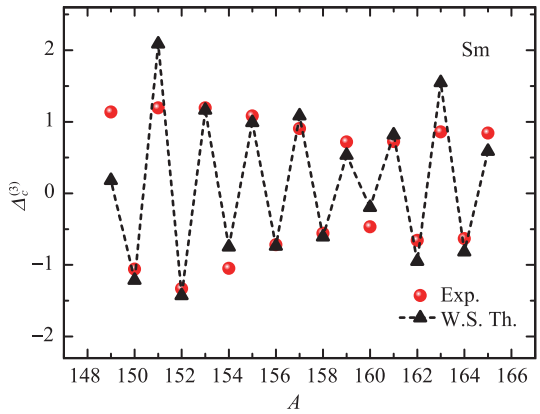

Fig. 4 (color online) The odd-even differences of $^{147-165}$Sm. Experimental values are denoted as "Exp.", which are taken from Ref. [21], the theoretical values calculated from the present model are denoted as "W.S.Th." and the pairing strength $G=0.06$ (MeV) .

5 Conclusion

A new iterative approach for solving the standard pairing problem is established based on a polynomial approach. It provides convenient initial guesses for both spherical and deformed systems, especially for large-size systems by using the Newton-Raphson algorithm with a Monte Carlo sampling procedure. It reduced the k-dimensional Monte Carlo sampling procedure to the one-dimensional Monte Carlo sampling procedure and avoid the non-solutions problem in Ref. [17] as well as the numerically unstable fluctuation in Ref. [16], which makes the computation significantly more efficient and reliable than traditional approaches. The advantage of the method makes the exact pairing solutions feasible for both the doubly-degenerate systems and degeneracies systems even when more energy levels or super-heavy nuclei are considered. The approach can easily be extended and applied to solve a large class of Gaudin-type quantum many-body problems. The results indicate that the present model can be used to explore the super-heavy nuclei and nuclear fission. Furthermore, it will be used to investigate the possible effects of pairing interaction on nuclear fission which may influence the prediction of the fission half-lives.

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标准对力模型的新迭代方法

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摘要： 建立了一种求解标准对力模型的新迭代方法。该方法基于标准对力模型的多项式方案，为球形和形变系统提供了方便的初始值预测。特别是对于大尺寸系统，该方法将求解 k 对多项式的系统方程式简化为分步求解 1 对多项式系统的迭代过程，并通过快速 Newton-Raphson 以及 Monte Carlo 采样算法逐步提供初始值预测。通过扩展，本算法还可用于解决 Gaudin 型量子多体问题，例如考虑超过 100 条轨道、50 对的大尺寸系统，以及超形变核、核裂变的研究中。

关键词： 标准对力模型；迭代近似；核裂变；超形变核

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