

The Heine-Stieltjes correspondence and the polynomial approach to the standard pairing problem

Feng Pan,^{1,2} Xin Guan,¹ Mingxia Xie,¹ Lina Bao,¹ and J. P. Draayer²

¹*Department of Physics, Liaoning Normal University, Dalian 116029, China*

²*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA*

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A new approach for solving the Bethe ansatz (Gaudin-Richardson) equations of the standard pairing problem is established based on the Heine-Stieltjes correspondence. For k pairs of valence nucleons on n different single-particle levels, it is found that solutions of the Bethe ansatz equations can be obtained from one $(k+1) \times (k+1)$ and one $(n-1) \times (k+1)$ matrices, which are associated with the extended Heine-Stieltjes and Van Vleck polynomials, respectively. Since the coefficients in these polynomials are free from divergence with variations in contrast to the original Bethe ansatz equations, the approach thus provides with a new efficient and systematic way to solve the problem, which, by extension, can also be used to solve a large class of Gaudin-type quantum many-body problems and to establish a new efficient angular momentum projection method for multi-particle systems.

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It is well known that the pairing force, similar to that in the Bardeen-Cooper-Schrieffer (BCS) theory of superconductors [1], as one of main residual interactions introduced to the nuclear shell model, is key to manifest ground state properties and low energy spectroscopy of nuclei, such as binding energies, odd-even effects, single-particle occupancies, excitation spectra, electromagnetic transition rates, beta-decay probabilities, transfer reaction amplitudes, low-lying collective modes, level densities, and moments of inertia, and so on [2]-[4]. Unlike electrons in solids, the drawbacks of the application of the BCS theory and its extensions to nuclei are noticeable 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 nonconservation (quasi-particle) approximations [5]-[6].

Exact solutions to the standard pairing problem was first obtained by Richardson, now referred to as the Richardson-Gaudin method [7]-[8]. Recently, extensions to the Richardson-Gaudin theory have also been made by using the Bethe ansatz methodology [9]-[12]. The advantage of the Richardson-Gaudin solutions lies in the fact that the huge matrix in the Fock subspace is reduced to a set of equations, of which the number equals exactly to that of pairs of valence particles involved. However, less attention had been paid to the Richardson's solutions of the pairing problem in realistic calculations mainly because the non-linear Bethe ansatz (Gaudin-Richardson) equations (BAEs) involved are very difficult to be solved numerically, especially for large size systems. Though there were a number of authors showing their efforts in designing algorithms for solutions with promising results [13]-[18], obviously efficient procedure for solving the problem seems still unclear. Thus, a simple and clear approach to the problem is in demand.

The Hamiltonian of the standard pairing model is

given by

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

where n is the total number of levels considered, $G > 0$ is the overall pairing strength, $\{\epsilon_j\}$ are unequal 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. Since the formalism for even-odd systems is similar, in the following, we only focus on the even-even seniority zero case. According to the Richardson-Gaudin method, k -pair eigenstates of (1) can be written as

$$|k; \zeta\rangle = S^+(x_1) S^+(x_2) \cdots S^+(x_k) |0\rangle, \quad (2)$$

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

$$1 - 2G \sum_j \frac{\rho_j}{x_i - 2\epsilon_j} - 2G \sum_{j(\neq i)} \frac{1}{x_i - x_j} = 0, \quad (3)$$

where $\rho_j = -(j+1/2)/2$, with the corresponding eigen-energy given by $E_n, k = \sum_{i=1}^k x_i$.

Actually, as shown by Heine and Stieltjes, there is a one-to-one correspondence between every set of the Gaudin-Richardson type equations (BAEs) and a set of orthogonal polynomials, called by us the extended Heine-Stieltjes polynomials. Roots of these BAEs are zeros

of the polynomials, which can be interpreted as stable equilibrium positions in two dimensional complex plane for a set of free unit charges in an external electrostatic field [19]. The link between Richardson's BCS pairing model for nuclei and the corresponding electrostatic problem was thus established [20]. According to Heine-Stieltjes correspondence, for nonzero pairing strength G , the polynomials $y(x)$ with zeros corresponding to the solutions of Eq. (3) should satisfy the following second-order Fuchsian equation:

$$A(x)y''(x) + B(x)y'(x) - V(x)y(x) = 0, \quad (4)$$

where $A(x) = \prod_{j=1}^n (x - 2\epsilon_j)$ is a polynomial of degree n , $B(x)$ is the polynomial with

$$B(x)/A(x) = \sum_{j=1}^n \frac{2\rho_j}{x - 2\epsilon_j} - \frac{1}{G}, \quad (5)$$

and $V(x)$ is called Van Vleck polynomials [19] of degree $n - 1$, which needs to be determined according to Eq. (4). In the original electrostatic analogue considered by Heine and Stieltjes [19], the parameters $\{\rho_j\}$ acting as fixed charges should all be positive with no external electrostatic field, $1/G \rightarrow 0$. Therefore, the polynomials $y(x)$ satisfying Eq. (4) with negative $\{\rho_j\}$ and $1/G \neq 0$ are thus called the extended Heine-Stieltjes polynomials, which tend to be the original Heine-Stieltjes polynomials with negative $\{\rho_j\}$ in the $G \rightarrow \infty$ limit.

In search for polynomial solutions of (4), we write

$$y(x) = \sum_{j=0}^k a_j x^j, \quad V(x) = \sum_{j=0}^{n-1} b_j x^j, \quad (6)$$

where $\{a_j\}$ and $\{b_j\}$ are the expansion coefficients to be determined. Substitution of (6) into Eq. (4) yields two matrix equations, the condition that coefficients in front of x^i ($i = 0, \dots, k$) must be zero generates a $(k + 1) \times (k + 1)$ matrix \mathbf{F} with $\mathbf{F}\mathbf{v} = b_0\mathbf{v}$, where the eigenvector \mathbf{v} of \mathbf{F} is just the expansion coefficients $\mathbf{v} = \{a_0, \dots, a_k\}$, while the condition that coefficients in front of x_i ($i = k + 1, \dots, n + k - 1$) must be zero generates another $(n - 1) \times (k + 1)$ upper-triangular matrix \mathbf{P} with $\mathbf{P}\mathbf{v} = 0$, which provides with unique solution of b_i ($i = 1, \dots, n - 1$) in terms of $\{a_j\}$. Entries of the two matrices are all linear with the coefficients $\{b_1, b_2, \dots, b_{n-1}\}$. Matrices \mathbf{F} and \mathbf{P} can easily be constructed, for which a simple MATHEMATICA code is provided [21].

Let the single-particle energies satisfy the interlacing condition $\epsilon_1 < \dots < \epsilon_n$. Real parts of zeros of $y(x)$ satisfy the interlacing condition, $-\infty < \mathbf{Re}(x_1) < \mathbf{Re}(x_2) < \dots < \mathbf{Re}(x_k) < +\infty$, where $\mathbf{Re}(x_i)$ lies in one of the $n + 1$ intervals $(-\infty, \epsilon_1)$, (ϵ_1, ϵ_2) , \dots , $(\epsilon_{n-1}, \epsilon_n)$, and $(\epsilon_n, +\infty)$. It should be noted that many $\mathbf{Re}(x_i)$ of adjacent zeros may lie within the same interval. When

$G \rightarrow \infty$, there will be only n intervals with $(-\infty, \epsilon_1)$ being removed. The number of different such allowed configurations gives the possible solutions of $y(x)$ and the corresponding $V(x)$. The number of solutions of $y(x)$, excluding those with sum of zeros of $y(x)$ complex, should equal to the number of levels produced by the standard pairing model, which is given by

$$\eta(n, k) = \sum_{p_1=0}^{-2\rho_1} \cdots \sum_{p_n=0}^{-2\rho_n} \delta_{q,k}, \quad (7)$$

where $q = \sum_{i=1}^n p_i$. When $\rho_i = -1/2$ for any i , which corresponds to the case of the Nilsson mean-field plus pairing model, $\eta(n, k) = n!/((n - k)!k!)$. Furthermore, if we set $a_k = 1$ in $y(x)$, the coefficient a_{k-1} must equal to negative sum of zeros of $y(x)$ with $a_{k-1} = -E_{n,k} = -\sum_{i=1}^k x_i$. Therefore, the solution corresponding to the largest real a_{k-1} is that for the ground state of the system considered; those corresponding to the next largest real a_{k-1} is that of the first excited state; and so on. In the standard pairing model, the solution with the same a_{k-1} is unique except complex conjugation and permutations within $\{x_i\}$, which will be helpful in simplifying the calculation process, especially when only a few low-lying states are needed in the application. Since the coefficients $\{a_j\}$ and $\{b_j\}$ in \mathbf{F} , \mathbf{P} , and \mathbf{v} are free from divergence with arbitrary variations in contrast to the original Bethe ansatz equations (3), one can use any standard recursive or iteration method to solve the problem with arbitrary initial values of these coefficients as desired. Because solving the eigen-equation $\mathbf{F}\mathbf{v} = b_0\mathbf{v}$, in which \mathbf{F} is a $(k + 1) \times (k + 1)$ matrix, is the only CPU time consuming operation involved, the CPU time needed in the process should always be reasonable for $k \sim 10^1 - 10^3$ and $n \sim 10^1 - 10^2$ sufficient to realistic applications in nuclear physics.

To demonstrate the new approach, we consider a simple example of $k = 5$ pairs in the sixth major shell with $n = 5$ levels, $1h_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$, and $1h_{11/2}$, which is related to the application of the solution to Sm isotopes [17], and difficult to be solved by directly using the BAEs (3). We set single-particle energies to be equal spacing with $\epsilon_i = i$, and the overall pairing strength $G = 0.5$. This example can now be dealt with easily by using the new polynomial approach, of which the number of solutions $y(x)$ is $\eta(5, 5) = 71$. First 5 sets of zeros of the corresponding polynomials $y(x)$ and the corresponding coefficient a_{k-1} are listed in Table I. The results can be obtained from the MATHEMATICA on a PC with in a minute. However, we observed there are some solutions with complex a_{k-1} , and some solutions are very close to each other like degenerate, which happened when MATHEMATICA built-in functions were used. Thus, the total number of solutions obtained is greater than $\eta(n, k)$, of which solutions with complex a_{k-1} should be

discarded. Because there is little to be known about these polynomials with negative charges, further study is needed to see whether there are indeed solutions with complex a_{k-1} . Both complex a_{k-1} and near degenerate issues may all be due to the Newtonian iteration adopted in the original MATHEMATICA package for solving a set of equations. Special codes designed suitable for the approach seem needed to overcome the ambiguity.

TABLE I: First 5 sets of zeros of the possible solutions of the extended Heine-Stieltjes polynomials and the corresponding eigen-energies (in arbitrary unit) of the standard pairing model Hamiltonian (1) in the case of $k = 5$ pairs in the sixth major shell with $n = 5$ single-particle levels $1h_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$, and $1h_{11/2}$. The single-particle energies used are $\epsilon_i = i$, and the overall pairing strength $G = 0.5$.

Zeros of the polynomials	$\sum_{i=1}^5 x_i$
$x_1 = -1.4993$, $x_2 = -1.1412 - 2.1396i$, $x_3 = -1.1412 + 2.1396i$, $x_4 = 0.0829 - 4.5018i$, $x_5 = 0.0829 + 4.5018i$	-3.6158
$x_1 = -0.5078 - 1.0411i$, $x_2 = -0.5078 + 1.0411i$, $x_3 = 0.5469 - 3.3066i$, $x_4 = 0.5469 + 3.3066i$, $x_5 = 2.9517$	3.0299
$x_1 = -0.9234 - 1.0718i$, $x_2 = -0.9234 + 1.0718i$, $x_3 = 0.0573 - 3.3613i$, $x_4 = 0.0573 + 3.3613i$, $x_5 = 5.2767$	3.5444
$x_1 = -1.1244 - 1.0987i$, $x_2 = -1.1244 + 1.0987i$, $x_3 = -0.1739 - 3.4422i$, $x_4 = -0.1739 + 3.4422i$, $x_5 = 7.4346$	4.8379
$x_1 = -1.2032 - 1.1109i$, $x_2 = -1.2032 + 1.1109i$, $x_3 = -0.2619 - 3.4804i$, $x_4 = -0.2619 + 3.4804i$, $x_5 = 8.7004$	5.77020

In addition, as shown in our previous study [22], a new angular momentum projection method for multi-particle systems can be established based on BAEs similar to (3). In fact, for n angular momenta j_i ($i = 1, 2, \dots, n$), the multi-particle state with total angular momentum $J = \sum_i j_i - k$ can be written as

$$|\eta, J, M = J\rangle = J^-(x_1)J^-(x_2)\cdots J^-(x_k)|\text{h.w.}\rangle, \quad (8)$$

where η is a quantum number needed to resolve the multi-occurrence of J , $|\text{h.w.}\rangle$ is the highest weight single-particle product state with $|j_1, m_1 = j_1, \dots, j_n, m_n = j_n\rangle$, and

$$J^-(x) = \sum_{i=1}^n \frac{1}{x - 2\epsilon_i} J_i^-, \quad (9)$$

in which J_i^- is the angular momentum lowering operator only acting on the i -th single-particle state $|j_i, m_i\rangle$,

and ϵ_i ($i = 1, 2, \dots, n$) can be taken as any set of unequal numbers [22]. Acting the total angular momentum raising operator J^+ to (8) with $J^+|\eta, J, M = J\rangle = 0$, one obtains the BAEs of $\{x_i\}$ the same as Eq. (3) in the replacement $\rho_i = -(j_i + 1/2)/2$ in the $G \rightarrow \infty$ limit. Therefore, once the solutions of (3) in the $G \rightarrow \infty$ limit are obtained, the resultant $\{x_i\}$ once and for all determine the multi-particle state with good angular momentum J . The number of solutions of (3) equals exactly to the number of occurrence of J for the given system. The polynomial solutions (4) in this case exactly become the Heine-Stieltjes polynomials mentioned previously. This angular momentum projection is certainly much simpler than the projection operator technique [3] and that based on the permutation group method [23].

In summary, we have established a new approach for solving the standard pairing problem based on a sound mathematical foundation — the extended Heine-Stieltjes polynomials and the corresponding Van Vleck polynomials satisfying the polynomial solutions of the second order Fuchsian equation. Thus, we reach the goal of the Richardson-Gaudin theory via the Heine-Stieltjes correspondence, from which the exact solutions to the problem can practically be realized based on two matrix equations. The approach can easily be extended and applied to solve a large class of Gaudin-type quantum many-body problems. A new efficient angular momentum projection method for multi-particle systems is thus proposed as a byproduct, of which the application to either boson or fermion systems will be studied elsewhere.

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- [1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
 - [2] S. T. Belyaev, Mat. Fys. Medd. Dan. Vid. Selsk. **31** (11) (1959).
 - [3] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer Verlag, Berlin, 1980).
 - [4] M. Hasegawa and S. Tazaki, Phys. Rev. C **47**, 188 (1993).
 - [5] A. K. Kerman and R. D. Lawson, Phys. Rev. **124**, 162 (1961).
 - [6] A. Volya, B. A. Brown, and V. Zelevinsky, Phys. Lett. B **509**, 37 (2001).
 - [7] R. W. Richardson, Phys. Lett. **3**, 277 (1963); **5**, 82 (1963); R. W. Richardson and N. Sherman, Nucl. Phys. **52**, 221 (1964); **52**, 253 (1964).
 - [8] M. Gaudin, J. Physique **37**, 1087 (1976).
 - [9] Feng Pan, J. P. Draayer, and W. E. Ormand, Phys. Lett.

- B **422**, 1 (1998); Feng Pan and J. P. Draayer, Phys. Lett. B **451**, 1 (1999); Feng Pan and J. P. Draayer, Phys. Rev. C **66**, 044314 (2002).
- [10] J. Dukelsky, C. Eсеbbag, and P. Schuck, Phys. Rev. Lett. **87**, 066403 (2001); G. Ortiz, R. Somma, J. Dukelsky and S. Rombouts, Nucl. Phys. B 707, **421** (2005); J. Dukelsky, V. G. Gueorguiev, P. Van Isacker, S. Dimitrova, B. Errea, and S. Lerma H., Phys. Rev. Lett. **96**, 072503 (2006).
- [11] H.-Q. Zhou, J. Links, R. H. McKenzie, and M. D. Gould, Phys. Rev. B **65**, 060502(R) (2002); J. Links, H.-Q. Zhou, R. H. McKenzie, and M. D. Gould, J. Phys. Math. Gen. A **36**, R63 (2003).
- [12] A. B. Balantekin, J. H. de Jesus, and Y. Pehlivan, Phys. Rev. C **75**, 064304 (2007); A. B. Balantekin and Y. Pehlivan, Phys. Rev. C **76**, 051001(R) (2007).
- [13] J. M. Roman, G. Sierra, and J. Dukelsky, Nucl. Phys. B **634**, 483 (2002).
- [14] S. Rombouts, D. Van Neck, and J. Dukelsky, Phys. Rev. C **69**, 061303(R) (2004)
- [15] F. Domínguez, C. Eсеbbag, and J. Dukelsky, J. Phys. A: Math. Gen. **39**, 11349 (2006).
- [16] M. Sambataro, Phys. Rev. C **75**, 054314 (2007).
- [17] G. G. Dussel, S. Pittel, J. Dukelsky, and P. Sarriguren, Phys. Rev. C **76**, 011302(R) (2007).
- [18] A. Faribault, O. El Araby, C. Sträter, and V. Gritsev, Phys. Rev. B **83**, 235124 (2011).
- [19] G. Szegő, *Amer. Math. Soc. Colloq. Publ. Vol. 23* (Amer Math Soc, Providence, RI, 1975)
- [20] J. Dukelsky, C. Eсеbbag, and S. Pittel, Phys. Rev. Lett. **88**, 062501 (2002).
- [21] Input $k, n, \epsilon[i], G,$ and $\rho[i]$. The rest code is the following: $y[x] = \text{Sum}[a[i] x^i, \{i, 0, k\}]$; $V[x] = \text{Sum}[b[i] x^i, \{i, 0, n - 1\}]$; $qq = \text{Expand}[\text{Simplify}[\text{Product}[(x - 2 \epsilon[i]), \{i, 1, n\}] \text{D}[\text{D}[y[x], x], x] + (\text{Expand}[\text{Product}[(x - 2 \epsilon[j]), \{j, 1, n\}] \text{Sum}[2 \rho[j]/(x - 2 \epsilon[j]), j, 1, n]]) \text{D}[y[x], x] - V[x] y[x]]]$; $x = 0$; $ss[0] = qq$; $\text{Clear}[x]$; $\text{Do}[ss[i] = \text{Coefficient}[qq, x^i], \{i, 1, n + k - 1\}]$; $st = \text{Flatten}[\text{Table}[ss[i], \{i, 0, n + k\}]]$; $ct = \text{Flatten}[\text{Table}[a[i], \{i, 0, k\}]]$; $F = \text{Table}[\text{Coefficient}[st[[i + 1]], ct[[j + 1]]], \{i, 0, k\}, \{j, 0, k\}]$; $P = \text{Table}[\text{Coefficient}[st[[i + 1]], ct[[j + 1]]], \{i, k + 1, n + k - 1\}, \{j, 0, k\}]$; $Pv = P.\text{Table}[a[i], \{i, 0, k\}]$; $\text{solb} = \text{Solve}[\text{Table}[Pv[[i]] == 0, \{i, 1, \text{Length}[Pv]\}], \text{Table}[b[i], \{i, 1, n - 1\}]]$; $vv = \text{Flatten}[\text{Table}[b[i], \{i, 1, n - 1\}] / . \text{solb}]$; $\text{Do}[b[i] = vv[[i]], \{i, 1, n - 1\}]$; $a[k] = 1$; $\text{rot} = \text{Flatten}[\{\text{Table}[a[i], \{i, 0, k - 1\}], b[0]\}]$; $Fv = F.\text{Table}[a[i], \{i, 0, k\}]$; $u = \text{NSolve}[\text{Table}[Fv[[i]] == 0, \{i, 1, k + 1\}], \text{rot}]$. The final results u provide with all solutions, in which those with sum of zeros complex should be discarded.
- [22] Feng Pan, Mo-Lin Ge, and J. P. Draayer, J. Phys. A: Math. Gen. **33**, 4917 (2000).
- [23] J. D. Louck and L. C. Biedenharn, *Lectuer Notes in Chemistry* **12**, (Springer, Berlin, 1979).