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2000 J. Phys. A: Math. Gen. 33 9095

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## Simple exact solutions of one-dimensional finite-chain hard-core Bose–Hubbard and Fermi–Hubbard models

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Received 21 March 2000, in final form 12 October 2000

**Abstract.** Exact algebraic solutions of a one-dimensional finite-chain hard-core Bose–Hubbard model with nearest-neighbour interactions, which is related to a state-dependent nuclear pairing interaction with a nearest-state interaction approximation, are derived based on a simple algebraic approach. Further extensions to arbitrary spin cases and the corresponding Fermi–Hubbard model are also presented.

The Bose–Hubbard model [1] has attracted theoretical and experimental interest of late because of its use in describing granular and short-correlation-length superconductors [2,3], Josephson junction arrays [4,5], and, most recently, cold atoms in optical lattices [6]. In each case, the relevant particles—Cooper pairs or lattice fluxes—are, at least approximately, bosonic. A similar situation occurs in the nuclear pairing problem in well-deformed nuclei, in which the pairing interactions can also be described by a finite-chain hard-core Bose–Hubbard model.

Up to a constant, the Hamiltonian of the one-dimensional finite-chain hard-core Bose–Hubbard model with nearest-neighbour hopping considered is

$$\hat{H} = \sum_{ij} t_{ij} \mathcal{P}_i b_i^\dagger b_j \mathcal{P}_j \tag{1}$$

where  $b_i^\dagger$ , and  $b_j$  are boson creation and annihilation operators, only  $t_{ii}$ ,  $t_{i+1}$  and  $t_{i+1i}$  are non-zero parameters and  $\mathcal{P}_i$  is a projection operator onto the subspace with no doubly occupied sites, which may be defined as

$$\mathcal{P}_i(\dots b_i^{\dagger n_i} \dots) = \begin{cases} 0 & \text{for } n_i \geq 2 \\ (\dots b_i^{\dagger n_i} \dots) & \text{otherwise} \end{cases} \tag{2}$$

where (...) represent other boson creation operators. In this paper, it will be shown that the finite-chain hard-core Bose–Hubbard Hamiltonian (1) can be solved by using a simpler algebraic method.

Up to a normalization constant, it is easy to prove that the eigenstates of (1) for a  $k$ -particle excitation can be expressed as

$$|k; \zeta\rangle = \sum_{i_1 < i_2 < \dots < i_k} C_{i_1 i_2, \dots, i_k}^{(\zeta)} b_{i_1}^\dagger b_{i_2}^\dagger \dots b_{i_k}^\dagger |0\rangle \tag{3}$$

where  $|0\rangle$  is the hard-core boson vacuum and  $C_{i_1 i_2 \dots i_k}^{(\zeta)}$  is a determinant given by

$$C_{i_1 i_2 \dots i_k}^{(\zeta)} = \begin{vmatrix} g_{i_1}^{\zeta_1} & g_{i_2}^{\zeta_1} & \dots & g_{i_k}^{\zeta_1} \\ g_{i_1}^{\zeta_2} & g_{i_2}^{\zeta_2} & \dots & g_{i_k}^{\zeta_2} \\ \dots & \dots & \dots & \dots \\ g_{i_1}^{\zeta_k} & g_{i_2}^{\zeta_k} & \dots & g_{i_k}^{\zeta_k} \end{vmatrix} \quad (4)$$

where  $\zeta$  is shorthand notation for a selected set of  $k$  eigenvalues of the  $t$  matrix, which can be used to distinguish the eigenstates with the same boson number  $k$ , and  $g^{\zeta_p}$  is the  $p$ th eigenvector of the  $t$  matrix. Eigenvalues  $E^{(\zeta_p)}$  of the  $t$  matrix and the corresponding eigenvector  $g^{\zeta_p}$  can be obtained from the eigen-equation

$$\sum_j t_{ij} g_j^{\zeta_p} = E^{(\zeta_p)} g_i^{\zeta_p}. \quad (5)$$

The corresponding excitation energies can be expressed as a sum of  $k$  different eigenvalues of the  $t$  matrix due to no double occupancy being allowed. Hence, the  $k$ -particle excitation energy is given by

$$E_k^{(\zeta)} = \sum_{j=1}^k E^{(\zeta_j)}. \quad (6)$$

One can easily check that equations (3)–(6) are valid when  $t$  is Hermitian, which is now assumed to be real for simplicity. Firstly, directly applying the Hamiltonian (1) on (3), one gets

$$\sum_p \sum_{i, i_1 < i_2 < \dots < i_k} C_{i_1 i_2 \dots i_k}^{(\zeta)} t_{i i_p} b_{i_1}^\dagger b_{i_2}^\dagger \dots b_{i_p \rightarrow i}^\dagger \dots b_{i_k}^\dagger |0\rangle \quad (7)$$

where  $i_p \rightarrow i$  means replacing the  $p$ th index  $i_p$  by  $i$ , there is no restriction on index  $i$  and, because of the projection operator  $\mathcal{P}$ , no two indices  $i_p$  and  $i_q$  among  $\{i_1, i_2, \dots, i_k\}$  can take the same value. The tri-diagonal condition on the hopping matrix  $t$ , the strict ordering of the indices in ansatz (3) and the projection operator  $\mathcal{P}$  together enforce that

$$i_{p-1} < i < i_{p+1}. \quad (8)$$

Once (8) is satisfied, other conditions will either be obviously satisfied or lead to zero terms in equation (7) because there is no pair of indices taking the same value among  $\{i_1, i_2, \dots, \}$  with  $\mu = i_p$  or  $\mu = i$ . Then, by eigen-equation, we have

$$\sum_{i_q} C_{i_1, \dots, i_{q-1} i_q i_{q+1}, \dots, i_k}^{(\zeta)} t_{i_\mu i_q} = \sum_P (-)^P E^{(\zeta_{P(\mu)})} g_{i_1}^{(\zeta_{P(1)})} g_{i_2}^{(\zeta_{P(2)})} \dots g_{i_\mu}^{(\zeta_{P(\mu)})} \dots g_{i_k}^{(\zeta_{P(k)})} \quad (9)$$

where  $P$  runs over all permutations  $(1, 2, \dots, k)$ ,  $E^{(\zeta_\mu)}$  is the  $\mu$ th eigenvalue of the  $t$  matrix and  $i_q$  in the summation can only be taken to be  $i_\mu, i_\mu \pm 1$ , because the nearest-hopping matrix is tri-diagonal. Hence, from equations (7) and (9) we finally get

$$\hat{H}|k; \zeta\rangle = \sum_{i_1 < i_2 < \dots < i_k} \sum_{\mu=1}^k \sum_P (-)^P E^{(\zeta_{P(\mu)})} \times g_{i_1}^{(\zeta_{P(1)})} g_{i_2}^{(\zeta_{P(2)})} \dots g_{i_\mu}^{(\zeta_{P(\mu)})} \dots g_{i_k}^{(\zeta_{P(k)})} b_{i_1}^\dagger b_{i_2}^\dagger \dots b_{i_k}^\dagger |0\rangle = E_k^{(\zeta)} |k; \zeta\rangle \quad (10)$$

which is valid for any  $k$ , where  $E_k^{(\zeta)}$  is still given by (6). It is clear that the wavefunctions given by (3) are free from doubly occupied sites. It seems from equations (7)–(10) that the coefficient  $C_{i_1 i_2 \dots i_k}^{(\zeta)}$  could either be a permanent or a determinant of  $g_{i_k}^{(\zeta_p)}$ . In fact, it should be a permanent with no restriction on summation indices if there is no projection operator involved in (1). Furthermore, it is well known that a permanent can be decomposed into sums

of symmetric, non-symmetric and totally antisymmetric parts with respect to permutation of indices. The non-antisymmetric components allow at least one pair of the indices among  $\{i_1, i_2, \dots, i_k\}$  to be the same, which must be the case if one takes the coefficient  $C_{i_1 i_2 \dots i_k}^{(\zeta)}$  symmetric with respect to permutation of the indices. However, because projection (2) is involved in Hamiltonian (1), other non-antisymmetric components must be set to zero. Hence, the only allowed components,  $C_{i_1 i_2 \dots i_k}^{(\zeta)}$ , in ansatz (3) are totally antisymmetric with respect to permutation of indices. The eigenstate equation (3) is obviously non-zero because the sum runs over the indices  $\{i_1, i_2, \dots, i_k\}$  with strict ordering.

If one assumes that the total number of sites is  $N$ , the  $k$ -particle excitation energies are determined by the sum of  $k$  different eigenvalues chosen from the  $N$  eigenvalues of the  $t$  matrix. Therefore, the total number of excited levels is  $N!/k!(N-k)!$ . Thus, the eigenvalue problem of the one-dimensional finite-chain hard-core Bose–Hubbard model, of which the effective Hamiltonian is given by (1), is simply solved.

The hard-core Bose–Hubbard model is also related to the nuclear pairing interaction. As is well known, a constant strength-pairing interaction, which is used in many applications, is not a particularly good approximation for well-deformed nuclei. In [7] a state-dependent Gaussian-type pairing interaction with

$$G_{\alpha\beta} = Ae^{-B(\epsilon_\alpha - \epsilon_\beta)^2} \quad (11)$$

was used, where  $\epsilon_\alpha$  and  $\epsilon_\beta$  represent, respectively, single-particle energies of states  $\alpha$  and  $\beta$ . The parameters  $A < 0$  and  $B > 0$  are adjusted in such a way that the location of the first excited eigensolution lies approximately at the same energy as for the constant pairing case. Of course, there is some freedom in adjusting the parameters, allowing one to control in a phenomenological manner the interaction among the states that differ by larger amounts in energy. Expression (11) allows one to model in a schematic way interactions between pairs of single-particle states ( $\alpha, \beta$ ) that lie closest in energy. The scattering between particles occupying such states will be favoured, whereas scattering between particles in states whose energies are greater than these will be reduced. As an approximation, such a pair interaction may be further simplified to the nearest-orbit interactions. Namely,  $G_{\alpha\beta}$  is given by (1) if two states  $\alpha$  and  $\beta$  lie closest in energy, with  $G_{\alpha\beta}$  taken to be 0 otherwise.

Let  $a_i^\dagger$  be the  $i$ th-orbital single-fermion creation operator, and  $a_i^\ddagger$  that of the corresponding time-reversed state. The fermion pairing operator can be expressed as

$$b_i^\dagger = a_i^\dagger a_i^\ddagger \quad b_i = a_i a_i \quad (12)$$

which satisfy the following deformed boson commutation relations [8]:

$$[b_i, b_j^\dagger] = \delta_{ij}(1 - 2N_i) \quad [N_i, b_j^\dagger] = \delta_{ij} b_j^\dagger \quad [N_i, b_j] = -\delta_{ij} b_j \quad (13)$$

where  $N_i = \frac{1}{2}(a_i^\dagger a_i + a_i^\ddagger a_i^\ddagger)$ , which is the pair number operator in  $i$ th orbit for even–even nuclei. Because, at most, only one fermion pair or a single fermion is allowed in each orbit due to the Pauli principle, these fermion pairs can equivalently be treated as exact bosons with projection onto the subspace with no doubly occupied orbits if only pure-pair dynamics is discussed. Hence, the pairing Hamiltonian in this case can be expressed as

$$\hat{H}_{\text{pairing}} = \sum_i' \epsilon_i + \sum_{ij} \mathcal{P} t_{ij} b_i^\dagger b_j \mathcal{P} \quad (14)$$

where the prime indicates that the sum runs over the orbits occupied by a single fermion which occurs in the description of odd- $A$  nuclei or broken pair cases, while these orbits should be excluded in the second sum,  $t_{ii} = 2\epsilon_i + G_{ii}$  with  $G_{ii} = A$  and  $\epsilon_i$  the single-particle energy,  $t_{ii+1} = t_{i+1i} = G_{ii+1}$ ,  $t_{ij} = 0$  otherwise. It is obvious that (14) is a special case of the one-dimensional hard-core Bose–Hubbard model [9], which differs from (1) only by a constant

term. Generally, the main difference is that the  $t$  matrix elements  $t_{ii+1}$  are all the same,  $t_{ii} = 0$ , for the former, while, generally,  $t_{ii+1}$  are different for different orbitals for the pairing model. Furthermore, the number of orbits in the nuclear pairing model is finite, while the number of sites in the Bose–Hubbard model is infinite with periodic condition, in general.

It is interesting to note that the above solutions of the eigenvalue problem of the hard-core Bose–Hubbard model can be extended to both hard-core Bose–Hubbard and Fermi–Hubbard models with arbitrary spin  $s$  for finite-site system, which leads to the following theorem.

**Theorem.** *The excitation energies of both the Bose– and the Fermi–Hubbard models of spin  $s$  with Hamiltonian given by*

$$\hat{H} = \sum_{ij} t_{ij} \mathcal{P} E_{ij} \mathcal{P} \tag{15}$$

where  $\mathcal{P}$  is a projection operator on the subspace with no doubly occupied sites,  $t_{ij} = t_{ii} \delta_{ji} + t_{ii+1} \delta_{ji+1} + t_{ii-1} \delta_{ji-1}$  with  $1 \leq i, j \leq N$  for finite-site system, and the  $U(N)$  generators

$$E_{ij} = \sum_{\sigma=-s}^s f_{i\sigma}^\dagger f_{j\sigma} \tag{16}$$

where  $f_{i\sigma}^\dagger$  is the  $i$ th-site boson or fermion creation operator with spin component  $\sigma$ , are given by a sum of  $k$  different eigenvalues chosen from the  $N$  eigenvalues of the  $t$  matrix in all possible ways:

$$E_k^{(\zeta)} = \sum_{i=1}^k E^{(\zeta_i)}. \tag{17}$$

The corresponding wavefunctions are given by

$$|k; \zeta, (\sigma_1 \sigma_2 \dots \sigma_k)\rangle = \sum_{i_1 < i_2 < \dots < i_k} C_{i_1 i_2 \dots i_k}^{(\zeta)} f_{i_1 \sigma_1}^\dagger f_{i_2 \sigma_2}^\dagger \dots f_{i_k \sigma_k}^\dagger |0\rangle \tag{18}$$

where the expansion coefficients  $C_{i_1 i_2 \dots i_k}^{(\zeta)}$  is given by the determinant (4) obtained according to equation (5) for the Bose or Fermi case.

Equation (18) can further be labelled by the  $U(2s + 1)$  group chains. For example, one can first rewrite (18) in terms of  $U(2s + 1) \supset U(2s) \supset \dots \supset U(1)$  canonical basis as

$$|k; \zeta, [\lambda_1, \lambda_2, \dots, \lambda_{2s+1}]w\rangle = \sum_{m; i_1 < i_2 < \dots < i_k} C_{i_1 i_2 \dots i_k}^{(\zeta)} a_m^{[\lambda]w} |Y_m^{[\lambda]}(\omega; w)\rangle \tag{19}$$

where  $[\lambda] \equiv [\lambda_1, \lambda_2, \dots, \lambda_{2s+1}]$  labels an irrep of  $U(2s + 1)$  and its conjugate irrep  $[\tilde{\lambda}]$  labels an irrep of  $U(N)$  simultaneously.  $m$  labels a special Gel'fand state of  $U(2s + 1)$  and the standard basis of the symmetric group  $S_k$  simultaneously [10],  $\omega \equiv (i_1, i_2, \dots, i_k)$  are indices of the corresponding boson or fermion creation operators,  $(\omega; w)$  stands for filling  $k$  different indices  $i_1, \dots, i_k$  into the Young tableau, after summing over these indices, substituting first  $f_1$  indices  $i_1, i_2, \dots, i_{f_1}$  in the tableau by  $\sigma_1$ , next  $f_2$  indices  $i_{f_1+1}, \dots, i_{f_2}$  in the tableau by  $\sigma_2$ , and so on, which results in a corresponding Weyl tableau  $w$  labelling the irrep  $[\lambda]$  in the canonical basis of  $U(2s + 1)$ , and  $a_m^{[\lambda]w}$  is the corresponding symmetrization coefficient [10] needed to map the special Gel'fand basis into a desired configuration  $[\lambda]w$  of the  $U(2s + 1)$  Gel'fand basis.

In this case, there are two duality relations involved.  $[\lambda]$  labels an irrep of  $U(2s + 1)$ , while its conjugate  $[\tilde{\lambda}]$  labels that of  $U(N)$ , because these two groups are in duality relation resulting from the branching rule  $U(N(2s + 1)) \downarrow U(N) \times U(2s + 1)$ . Furthermore, an irrep  $[\lambda]$ , with a Young diagram consisting of  $k$  boxes, of the symmetric group  $S_k$ , is also the same irrep of  $U(2s + 1)$  because of the Schur–Weyl duality relation between the symmetric group

$S_k$  and the unitary group  $U(2s+1)$  [10, 11]. One can then construct the standard basis  $Y_m^{[\lambda]}(\omega)$  of the symmetric group  $S_k$ , where  $Y_m^{[\lambda]}(\omega)$  is the Young tableau, and  $m$  is the index of the tableau. It has been proven [11] that the standard basis  $Y_m^{[\lambda]}$  of  $S_k$  is also a special Gel'fand basis of  $U(2s+1)$ . In order to obtain a general Gel'fand basis labelled by the corresponding Weyl tableau  $[\lambda](w)$  of  $U(2s+1)$  from the standard basis of symmetric group  $S_k$ , one needs to replace  $f_1$  indices  $i_1, i_2, \dots, i_{f_1}$  by  $\sigma_1$ , and  $f_2$  indices  $i_{f_1+1}, \dots, i_{f_2}$  by  $\sigma_2$ , and so on. Then, after the symmetrization, one obtains a desired Gel'fand basis of  $U(2s+1)$  labelled by  $[\lambda]w$ . This procedure for obtaining the special Gel'fand basis  $|Y_m^{[\lambda]}(\omega)\rangle$  from the  $k$ -particle product state  $f_{i_1\sigma_1}^\dagger f_{i_2\sigma_2}^\dagger \dots f_{i_k\sigma_k}^\dagger |0\rangle$  was outlined in [11].

The total spin  $S$  and its third component  $S_0$  of the system can be determined by the branching rule of  $U(2s+1) \supset SU(2) \supset U(1)$  with branching multiplicity  $\tau$  of  $U(2s+1) \supset SU(2)$ . The final state with  $S$  and  $S_0$  being good quantum numbers can be obtained from (19) through state transformation:

$$|k, \zeta; [\lambda]\tau SS_0\rangle = \sum_w B_w^{\tau SS_0} |k, \zeta; [\lambda] w\rangle \quad (20)$$

where  $B_w^{\tau SS_0}$  is a matrix element of the transformation between the Gel'fand basis of  $U(2s+1)$  and the basis of  $U(2s+1) \supset SU(2) \supset U(1)$ .

The above theorem indicates that the one-dimensional finite-chain hard-core Hubbard models with nearest-neighbour hopping for both the Bose and Fermi cases have the same feature except for the permutation symmetry with respect to site exchange.

In summary, simple exact algebraic solutions of the one-dimensional finite-chain hard-core Bose–Hubbard model, which is related to the state-dependent nuclear pairing interaction with a nearest-orbit interaction approximation, have been derived. These results may be useful for understanding physical properties of the nuclear pairing in well-deformed nuclei. It has been shown that the excitation spectra and corresponding wavefunctions of the Bose–Hubbard model are identical to those of the corresponding Fermi–Hubbard model except for the site permutation. The results can easily be extended to arbitrary spin cases. In the pairing interaction for well-deformed nuclei, one still needs to check whether the nearest-orbit interaction is a good approximation or not. It is expected that the nearest-state interaction can be applied, at least to some well-deformed regions in which the parameter  $B$  in (11) is not small and the single-particle levels are well separated. Research work in this direction is in progress. On the other hand, though there are formulae for exact solutions of the nuclear pairing interaction for many cases [12–17] based on nonlinear Bethe equations, to solve these nonlinear equations is time consuming and not easy when the number of excited pairs  $k$  and total number of orbitals  $N$  are large, which is often the case for well-deformed nuclei. Nevertheless, numerical calculation of the eigenvalue problem (5) is simple and fast, from which the results determine all the excitation energies and the corresponding wavefunctions for any  $k$  according to equations (3)–(6). The results provide another limit situation, in contrast to the constant strength pairing approximation. In addition, the model can easily be used to test various approximation methods for solving the same problem.

## Acknowledgments

This work was supported by the US National Science Foundation through a regular grant, no 9970769, and a Cooperative Agreement, no EPS-9720652, which includes matching funding from the Louisiana Board of Regents Support Fund and the Science Foundation of the Liaoning Education Commission no 990311011.

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