Exactly solvable site-dependent Hubbard model

Feng Pan* and J. P. Draayer
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001
(Received 28 October 1998)

Exact solutions for the eigenvalue problem of a Hubbard model with special site-dependent t and U parameters is derived using an infinite-dimensional algebraic approach based on the Bethe ansatz.
[S0163-1829(99)05007-9]

As is well known, the Hubbard model[1,2] is used in the study of magnetic metallic materials. The success of the theory is due to its simplicity and rich physical content. It is also known that the so-called t-J model,[3] which is used for some high-T_c superconductors, is the strong correlation limit of the Hubbard model.[4] In general, the hopping terms t and the interaction parameters U should be chosen to be nonzero for any pair of sites. But when this is done the model is very difficult to solve. Explicit analytical results have only been obtained for a one-dimensional chain with nearest-neighbor interactions and constant t and U strengths using the coordinate Bethe ansatz,[5] the quantum inverse scattering method,[6–9] its SO(4) invariance,[10–12] Yangian symmetries,[13,14] and recent developments based on the algebraic and analytic Bethe ansatz. Recently, Bracken *et al.*[15] and Gould *et al.*[16] have studied quantum superalgebra to obtain a new extension of the Hubbard model with exact solutions.[17,18] In Ref. 19, a special t-J system, one that corresponds to an infinite U Hubbard model with constant t and J values between sites, was studied using a symmetric group approach. The ground-state configuration of the t-J system is known,[20] and a form for the general solution has been conjectured based on the spectra obtained through exact diagonalizations. Kirson exploited the supersymmetry of the model to derive analytical results for energy spectra, including degeneracies.[21]

In this paper, another special Hubbard U model is considered, one with site-dependent t and U parameters. In this case the Hamiltonian can be written as

$$H=\alpha\sum_{i,j,\sigma} t_{ij}^{\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i,j} U_{ij}n_{i\uparrow}n_{j\downarrow}, \tag{1}$$

where α can be ± 1. It will be shown that Hamiltonian (1) is exactly solvable under the following parameter separability assumptions:

$$t_{ij}^{\sigma}=\begin{cases} t_i^{\sigma}(t_j^{\sigma})^* & \text{for} \quad i\neq j, \\ \epsilon_i^{\sigma}+|t_i^{\sigma}|^2 & \text{for} \quad i=j, \end{cases} \tag{2a}$$

and

$$U_{ij}=\beta(\epsilon_i^{\uparrow}+\epsilon_j^{\downarrow}), \tag{2b}$$

where β is a real parameter. If the t parameters are spin-component dependent, the total spin of the system is not conserved, only the total number of electrons N and the third component of the spin are good quantum numbers.

This choice for the t_{ij}^{σ} parameters assigns a pairwise site-dependent value to the hopping term. A common choice is to set the t_i^{σ} all equal or all zero except for equal-strength nearest-neighbor interactions. Different t_i^{σ} can be used to bias the system towards a perferred configuration. From Eq. (2a) it follows that the ϵ_i^{σ} adds to (<0) or subtracts from (>0) the strength to the self-site t_{ii}^{σ} interaction terms in the Hamiltonian. In a standard Hubbard model theory the U_{ii} is taken to represent the on-site Coulomb repulsion, while other long-range terms with $i\neq j$ are neglected. In contrast, the U_{ij} with $i\neq j$ terms given by Eq. (2b) may exaggerate the long-range Coulomb interaction strength. This work demonstrates that the latter scenario is exactly solvable.

To diagonalize Hamiltonian (1), we introduce the operators

$$A_{n\sigma}^{+}=\sum_j (\epsilon_j^{\sigma})^n t_j^{\sigma}c_{j\sigma}^{\dagger}, \quad A_{n\sigma}=\sum_j (\epsilon_j^{\sigma})^n t_j^{\sigma *}c_{j\sigma},$$

$$\mathcal{N}_{n\sigma}=\sum_j (\epsilon_j^{\sigma})^n c_{j\sigma}^{\dagger}c_{j\sigma}, \quad n=0,1,2,\ldots, \tag{3}$$

which satisfy the anticommutation relations

$$[A_{n\sigma}^{+},A_{m\sigma'}]_{+}=\delta_{\sigma\sigma'}L_{m+n}^{\sigma}, \quad [A_{n\sigma}^{+},A_{m\sigma'}^{+}]_{+}=0,$$
$$[A_{n\sigma},A_{m\sigma'}]_{+}=0, \tag{4a}$$

and the commutation relations

$$[\mathcal{N}_{n\sigma},A_{m\sigma'}^{+}]=\delta_{\sigma\sigma'}A_{m+n\sigma}^{+}, \quad [\mathcal{N}_{n\sigma},A_{m\sigma'}]=-\delta_{\sigma\sigma'}A_{m+n\sigma}, \tag{4b}$$

where

$$L_n^{\sigma}=\sum_j (\epsilon_j^{\sigma})^n|t_j^{\sigma}|^2 \tag{5}$$

is an n-dependent c number. The algebra generated by $A_{n\sigma}^{+}$, $A_{n\sigma}$, and $\mathcal{N}_{n\sigma}$ with $n=0,1,2,\ldots$ is called a half-infinite-dimensional fermion algebra.

The lowest weight state of this system is the electron vacuum, $|0\rangle$, which satisfies

$$A_{n\sigma}|0\rangle=0. \tag{6}$$

Let u and d be the number of up and down spins, respectively. A general $u+p$ particle state, up to a normalization factor, can then be written as

$$|N\rangle = A_\uparrow^+(x_1)A_\uparrow^+(x_2)\cdots A_\uparrow^+(x_u)A_\downarrow^+(y_1) \times A_\downarrow^+(y_2)\cdots A_\downarrow^+(y_d)|0\rangle, \tag{7}$$

where $N=u+p$. It is assumed that the operator $A_\sigma^+(x_i)$ can be expanded in terms of the $A_{n\sigma}^+$ near $x_i \sim 0$, namely,

$$A_\sigma^+(x_i) = \sum_{n_i} a_{n_i\sigma} x_i^{n_i} A_{n_i\sigma}^+, \tag{8}$$

where

$$a_{n_i\sigma} A_{n_i\sigma}^+ = \frac{1}{2\pi i} \oint_0 dx_i x_i^{n_i} A_\sigma^+(x_i) \tag{9}$$

is the Fourier-Laurent coefficient in the expansion of $A_\sigma^+(x_i)$. It follows that the Bethe ansatz wave function (7) near $x_i \sim 0$ can be written as

$$|N\rangle = \sum_{n_i m_i} \prod_{k=1}^{u} a_{n_k\uparrow} x_k^{n_k} A_{n_k\uparrow}^+ \prod_{k'=1}^{d} a_{m_{k'}\downarrow} y_{k'}^{m_{k'}} A_{m_{k'}\downarrow}^+ |0\rangle. \tag{10}$$

Using Eq. (10) with relations (4a) and (4b), one can prove that the x_i with $i=1,2,\ldots,u$, and the y_j with $j=1,2,\ldots,d$, satisfy

$$\frac{\alpha+\beta d}{x_i} = \sum_k \frac{\alpha|t_k^\uparrow|^2}{1-\epsilon_k^\uparrow x_i}, \frac{\alpha+\beta u}{y_i} = \sum_k \frac{\alpha|t_k^\downarrow|^2}{1-\epsilon_k^\downarrow y_i}, \tag{11}$$

while the energy eigenvalue for the $N=u+d$ electrons is given by

$$E_N = (\alpha+\beta d)\sum_{i=1}^{u} \frac{1}{x_i} + (\alpha+\beta u)\sum_{i=1}^{d} \frac{1}{y_i}. \tag{12}$$

The eigenvalue of S_0 is simply $\frac{1}{2}(u-d)$.

Though these relations were derived for x_i and y_i near zero, by analytic continuation they are valid over the entire complex plane. We also find that the coefficients $a_{n_i\sigma}$ in Eq. (10) are n_i and σ independent. Hence, up to a constant, $A_\sigma^+(z_i)$ is of the form

$$A_\sigma^+(z_i) = \sum_j \frac{t_j^\sigma}{1-\epsilon_j^\sigma z_i} c_{j\sigma}^+. \tag{13}$$

It should be clear that wave function (7) is antisymmetric under permutations of the roots x_i or y_i. Furthermore, it follows from this that the roots x_i or y_i in Eq. (11) must all be distinct. Indeed, it can be verified from Eq. (11) that the roots are all different for up-spin or down-spin electrons, respectively, when the ϵ_i^σ, $i=1,2,\ldots$, are all different real numbers. In this case, one can arrange the roots for up-spin or down-spin as $|z_1|<|z_2|<\cdots<|z_u|<|z_p|$, where $p=u$ or d. There is no degeneracy for any root:

$$\frac{1}{z_i} = \sum_k \frac{|t_k^\sigma|^2}{1-\epsilon_k^\sigma z_i} \text{ for } i=1,2,\cdots,u \text{ when } \sigma=\uparrow \text{ or } d \text{ when } \sigma=\downarrow. \tag{14}$$

When the parameters t and ϵ are all σ independent, it can be proven that Hamiltonian (1) commutes with the total spin operators S_μ with $\mu=0,+,-$, defined by

$$S_+ = \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}, S_- = \sum_i c_{i\downarrow}^\dagger c_{i\uparrow}, S_0 = \frac{1}{2}\sum_i (n_{i\downarrow}-n_{i\uparrow}), \tag{15}$$

as well as the total electron number operator $N=N_\downarrow+N_\uparrow$, where

$$N_\uparrow = \sum_i n_{i\uparrow}, \quad N_\downarrow = \sum_i n_{i\downarrow}. \tag{16}$$

It follows that the total spin S and number operator are then good quantum numbers.

To construct eigenstates of the total spin in this case, one can start from the highest weight state,

$$|N, S=\tfrac{1}{2}N, S_0=S\rangle = A_\uparrow^+(z_1)A_\uparrow^+(z_2)\cdots A_\uparrow^+(z_N)|0\rangle, \tag{17}$$

which satisfies

$$S_+ A_\uparrow^+(z_1)A_\uparrow^+(z_2)\cdots A_\uparrow^+(z_N)|0\rangle = 0, \tag{18a}$$

and

$$S^2 A_\uparrow^+(z_1)A_\uparrow^+(z_2)\cdots A_\uparrow^+(z_N)|0\rangle = \tfrac{1}{2}N(\tfrac{1}{2}N+1)A_\uparrow^+(z_1)A_\uparrow^+(z_2)\cdots A_\uparrow^+(z_N)|0\rangle. \tag{18b}$$

Applying S_- in Eq. (17) $N/2-S_0$ times, yields, up to a normalization factor,

$$|N, S=N/2, S_0\rangle = (S_-)^{N/2-S_0}|N, S=\tfrac{1}{2}N, S_0=S\rangle \tag{19}$$

with energy eigenvalue of Hamiltonian (1) given by

$$E_{NS=N/2} = (\alpha+\beta N)\sum_{i=1}^{N} \frac{1}{z_i}, \tag{20}$$

where the z_i with $i=1,2,\ldots,N$ must satisfy

$$\alpha+\beta N = \sum_k \frac{\alpha|t_k|^2 z_i}{1-\epsilon_k z_i}. \tag{21}$$

Therefore, for N electrons and total spin $S=N/2$ the energy eigenvalue is $(N+1)$-fold degenerate with $S_0=N/2, N/2-1, \ldots, -N/2$.

A special state is the one with $S=0$ and $N=2$, which can be expressed as

$$P^0(z_1,z_2)|0\rangle = (A_\uparrow^+(z_1)A_\downarrow^+(z_2)+A_\uparrow^+(z_2)A_\downarrow^+(z_1))|0\rangle. \tag{22}$$

It should be noted that in Eq. (22) $z_1 \neq z_2$ because of the Pauli principle. Using the pairing operator $P^0(z_i,z_j)$, one can construct the following state with $N=2S+2k$:

$$|N=2S+2k,S,S_0\rangle=P^0(z_1,z_2)P^0(z_3,z_4)\cdots P^0(z_{2k-1},z_{2k}) \times(S_-)^{S-S_0}|2S,S,S\rangle, \quad (23)$$

where

$$|2S,S,S\rangle=A_\uparrow^+(z_{2k+1})A_\uparrow^+(z_{2k+2})\cdots A_\uparrow^+(z_{2k+2S})|0\rangle. \quad (24)$$

The eigenvalue $E_{N,S}$ of Hamiltonian (1) for any spin, when t and ϵ are σ independent, is still given by Eq. (20). All the c-numbers z_i in Eqs. (23) and (24) should satisfy Eq. (21).

It can be verified that some of the roots z_i in the product

$$P^0(z_1,z_2)P^0(z_3,z_4)\cdots P^0(z_{2k-1},z_{2k}) \quad (25)$$

can be the same. To understand the overall structure of the solutions better, first note that the roots in Eq. (24) should all be different. Furthermore, if the number of sites is L, the total number of different solutions of Eq. (21) is $L!/(L-2S)!(2S)!$ each $(2S+1)$-fold degenerate. Further degeneracy may enter through the pairing part, Eq. (25), of the wave function. For example, if z_1,z_2,z_3,z_4 are roots, the four-particle pairing part (25) can be taken as $P^0(z_1,z_2)P^0(z_3,z_4)$, $P^0(z_1,z_3)P^0(z_2,z_4)$, or $P^0(z_1,z_4)P^0(z_2,z_3)$. All of these have the same eigenenergy. Furthermore, if a root z_j does not enter in Eq. (24), it may occur twice in Eq. (25) in the following form:

$$\cdots P^0(z_i,z_l)P^0(z_i,z_m)\cdots; \quad (26)$$

whereas if z_i is used in Eq. (24), it can only occur in Eq. (25) once. For example, if z_1 is not taken by Eq. (24), while z_2, z_3, and z_4 are, the four-particle pairing part of the wavefunction can further be taken as $P^0(z_1,z_2)P^0(z_1,z_3)$, $P^0(z_1,z_2)P^0(z_1,z_4)$, or $P^0(z_1,z_3)P^0(z_1,z_4)$. The situation becomes more complicated with increasing number of spin zero pairs.

To summarize, exact solutions for the eigenvalue problem of a Hubbard U model, ones with separable t parameters and a simple site-dependent form for U, have been derived using an infinite-dimensional algebraic approach based on the Bethe ansatz. The Hubbard U model with spin-dependent t parameters and special site-dependent U parameters have also been discussed. The complete spectrum and the corresponding eigenstates are derived. Obviously, the Hubbard Hamiltonian (1) has three different phases: (i) when all parameters t_j^σ, and ε_j^σ are the same; (ii) when all these parameters are different; and (iii) when the parameter $\beta\to\infty$. The phase transition occurs when these parameters vary from one regime to another. In case (i) the solutions are particularly simple; and the pairing structure described in Eq. (23) will be totally missing becasue there only exists one root of Bethe equation (23). Therefore, the total number of electrons cannot exceed $2L$, where L is the number of sites, because of the Pauli principle. In case (ii) there are a sufficient number of solutions to Eq. (23), which leads to a rich structure of both the whole spectrum and the corresponding eigenstates as given by Eqs. (20)–(23). In case (iii) the Hubbard model considered will become a site-dependent t-J model, of which a site independent case was studied in detail in Ref. 21. In this case the double occupancy of any site is not allowed because of the infinite repulsion. Hence, its spectrum and eigenstates will be different from what are reported in this paper. The present results apply to the case of limit of zero electron correlation as well,[24] which is useful in the so-called pseudospin-electron model introduced at the consideration of the anharmonicity effects in high-T_c superconductors when the hopping parameters are assumed to be site dependent and separable.

It can be inferred from these results that the Hubbard U model Hamiltonian,

$$H=\alpha\sum_{i,j} t_{ij}c_{i\sigma}^\dagger c_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}, \quad (27)$$

can be easily diagonalized when $S=N/2$, yielding eigenenergies

$$E_{NS=N/2}=\alpha\sum_{i=1}^N \frac{1}{z_i} \quad (28)$$

under the Bethe ansatz (19), where the c numbers z_i satisfy

$$\frac{1}{z_i}=\sum_k \frac{|t_k|^2}{1-\epsilon_k z_i}. \quad (29)$$

The method can also be applied to other many-fermion interacting systems, such as the nuclear pairing problem.[22] The advantage of this method is that the building blocks $A_\sigma^+(z_i)$ of the Bethe ansatz wave functions can be derived. These building blocks satisfy a nonlinear fermion algebra of the Gaudin type[23]—an infinite dimensional algebra, which, generally, is an affine Lie algebra without central extension—which is the infinitesimal form of the corresponding nonlinear fermion algebra.

Supported by the National Science Foundation under Grant No. 9603006 and Cooperative Agreement No. EPS-9550481, which includes matching from the Louisiana Board of Regents Support Fund.

*On leave from the Department of Physics, Liaoning Normal University, Dalian 116029, P.R. China.

[1] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).
[2] J. Hubbard, Proc. R. Soc. London, Ser. A **277**, 237 (1964).
[3] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[4] K. A. Chao, J. Spalek, and A. M. Oles, J. Phys. C **10**, L271 (1977); C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987); Yu A. Izyumov, Usp. Fiz. Nauk **167**, 465 (1997) [Phys. Usp. **40**, 445, (1997)].
[5] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[6] B. S. Shastry, Phys. Rev. Lett. **56**, 1529 (1986); **56**, 2453 (1986).
[7] B. S. Shastry, J. Stat. Phys. **50**, 57 (1988).
[8] E. Olmedilla and M. Wadati, Phys. Rev. Lett. **60**, 1595 (1988).
[9] E. Olmedilla, M. Wadati, and Y. Akutsu, J. Phys. Soc. Jpn. **56**, 2298 (1987).
[10] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).
[11] F. H. L. Eßler, V. E. Korepin, and K. Schoutens, Phys. Rev. Lett. **67**, 3848 (1991).
[12] F. H. L. Eßler and V. E. Korepin, Phys. Rev. Lett. **72**, 908 (1994).

[13] D. B. Uglov, and V. E. Korepin, Phys. Lett. A **190**, 238 (1994).
[14] S. Murakami, J. Phys. A **31**, 6367 (1998).
[15] A. J. Bracken, M. D. Gould, J. R. Links, and Y. Z. Zhang, Phys. Rev. Lett. **74**, 2768 (1995).
[16] M. D. Gould, K. E. Hibberd, J. R. Links, and Y. Z. Zhang, Phys. Lett. A **212**, 156 (1996).
[17] P. B. Ramos and M. J. Martins, J. Phys. A **30**, 849 (1997).
[18] R. Yue and T. Deguchi, J. Phys. A **30**, 849 (1997).
[19] B. Binz, X. Zotos, and D. Baeriswyl, J. Phys. A **31**, 4225 (1998).
[20] J. A. Verges, F. Guinea, J. Galan, P. van Dongen, G. Chiappe, and E. Louis, Phys. Rev. B **49**, 15 400 (1994).
[21] M. W. Kirson, Phys. Rev. Lett. **78**, 4241 (1997).
[22] Feng Pan, J. P. Draayer, and W. E. Ormand, Phys. Lett. B **422**, 1 (1998).
[23] M. Gaudin, J. Phys. (France) **37**, 1087 (1976).
[24] K. A. Müller, Z. Phys. B **80**, 193 (1990).