Ground state and excitations of a four-component fermion model

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The properties of the ground state and excitations of a four-component Hubbard-like model are studied by the Lieb-Schultz-Mattis approach. It is proven rigorously that the ground state of the model is nondegenerate and excitations are gapless at all band fillings.

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The nature of the ground state and excitations of strongly correlated electronic systems plays an important role in our understanding of various fascinating phenomena such as metal-insulator transition, high-temperature superconductivity, and colossal magnetoresistance. Recently, there has been much interest in the studies of correlated electrons with orbital degree of freedom.[1] In the case of double orbital degeneracy, a SU(4) theory was proposed as an ideal limit.[2]

Although few rigorous results exist for general many-body Hamiltonians, significant progress has been made in one spatial dimension. In 1961, Lieb, Schultz, and Mattis (LSM) proved[3] a remarkable theorem: For the spin-$1/2$ Heisenberg antiferromagnetic chain, the ground state is nondegenerate and the energy spectrum is gapless. This theorem has been extended recently to a hierarchy of generalized Heisenberg models[4,5] with high ranking symmetries, including the SU(4) model. It is of interest to obtain results for systems where the kinetic terms caused by nearest-neighbor hopping is not negligible. For the two-component Hubbard model, the nondegeneracy of the ground state was shown by Lieb[6] and gaplessness at $1/2$ filling by Yamanaka, Oshikawa, and Affleck (YOA).[7] The extension of these results to four-component Hubbard-type models is valuable because such models not only describe electrons with double orbital degeneracy but also two layer systems without interlayer hopping. Experimental realization of the four-component or two-band Hubbard model in one dimension includes quasi-one-dimensional materials such as $Na_2Ti_2Sb_2O$ and NaV_2O_5.[8]

In this work, we consider a four-component Hubbard model defined on a one-dimensional lattice with length L,

$$H = -t \sum_{\substack{a \\ \langle x,x' \rangle}} c_a^+(x) c_a(x') + U \sum_{\substack{a<a' \\ x}} n_a(x) n_{a'}(x) + V \sum_{\substack{a,a' \\ \langle x,x' \rangle}} n_a(x) n_{a'}(x'), \quad (1)$$

where $a, a' = 1,2,3,4$; x identifies the lattice site, and $\langle x, x' \rangle$ stands for nearest-neighbor sites. $c_a^+(x)$ creates a fermion of component a on site x, and $n_a(x) = c_a^+(x) c_a(x)$ is the corresponding number operator. The on-site interaction is assumed to be repulsive. The four components can be related to electrons with doubly orbital degeneracy. Let us define the spin components by up ($\uparrow$) and down ($\downarrow$) and the orbital components by top and bottom. Then the four possible electron singly occupied states are

$$|1\rangle = \left| \begin{matrix} \uparrow \\ - \end{matrix} \right\rangle, |2\rangle = \left| \begin{matrix} \downarrow \\ - \end{matrix} \right\rangle, |3\rangle = \left| \begin{matrix} - \\ \uparrow \end{matrix} \right\rangle, |4\rangle = \left| \begin{matrix} - \\ \downarrow \end{matrix} \right\rangle.$$

Previous literature on such systems has largely concentrated on the strong-coupling limit of this Hamiltonian, whereby it is mapped onto a SU(4) Heisenberg model[9,10] and related models away from SU(4) symmetry.[11,12] For the SU(4) Heisenberg Hamiltonian, it has been established that there are gapless excitations at crystal momentum $K = \pm \pi/2$ and π.[2,9,10] In the case of no orbital degeneracy, it is well known that due to the existence of the charge gap for any $U > 0$, the low-energy physics of the Hubbard model is essentially identical to the SU(2) Heisenberg model. It is of interest to investigate if this is the case for the SU(4) case also. In particular, much insight can be obtained if exact and rigorous results are available to complement approximate results using methods like Bosonization.[13]

In the following, we first prove that the ground state of the Hamiltonian (1) with periodic boundary condition is nondegenerate when the total number of electrons is $N = 4n$ with n being an odd integer. We then study whether the excitations are gapless for different band filling.

To show nondegeneracy of the ground state, we shall apply a simplified version of Lieb and Mattis' method in proving the absence of ferromagnetism in one-dimensional itinerant electron lattice models.[14,15] First, we notice that, according to the representation theory of Lie algebra A_3, for any multiplet, there is always one state lying in the subspace of zero weight (0, 0, 0), which is spanned by the vectors with equal number of different kinds of fermions. Therefore, by introducing operators $\hat{\mathcal{C}}_a^\dagger(\mathbf{x}) = c_a^\dagger(x_1) c_a^\dagger(x_2) \cdots c_a^\dagger(x_n)$ with $x_1 < x_2 < \cdots < x_n$, we can write the ground-state wave-function as

$$|\psi_0\rangle = \sum_{\mu} W_\mu \hat{\mathcal{C}}_1^\dagger(\mathbf{x}) \hat{\mathcal{C}}_2^\dagger(\mathbf{x}') \hat{\mathcal{C}}_3^\dagger(\mathbf{x}'') \hat{\mathcal{C}}_4^\dagger(\mathbf{x}''') |0\rangle, \quad (2)$$

where μ stands for the set $\{\mathbf{x}, \mathbf{x}', \mathbf{x}'', \mathbf{x}'''\}$. Obviously, ψ_0 belongs to the subspace $V_0(n)$, in which each vector has the same number n of $a=1$, 2, 3, and 4 types of fermions. The total number of expansion terms in Eq. (2) is (C_L^n).[4]

In terms of this basis of vectors, we are able to write Hamiltonian (1) into a matrix $\mathcal{H}$ which has the following characteristics: (i) All of its off-diagonal elements are either zero or $-t$, although its diagonal elements may have different signs. The reason why off-diagonal elements all have the same sign is due to the fact that, in Hamiltonian (1), only hopping terms between nearest-neighbor sites are present. In one dimension, such hopping will not change the positional order of the fermions except at the boundary. However, if the periodic boundary condition is used for n odd, then the boundary hopping will not cause sign problems. (ii) Furthermore, $\mathcal{H}$ is also irreducible. Namely, for any pair of indices m and n, there is a positive integer M such that the matrix element $(\mathcal{H}^M)_{mn}$ is nonzero since the chain is connected by fermion hopping. Therefore any pair of configurations $\hat{\mathcal{C}}_1^\dagger(\mathbf{x})\hat{\mathcal{C}}_2^\dagger(\mathbf{x}')\hat{\mathcal{C}}_3^\dagger(\mathbf{x}'')\hat{\mathcal{C}}_4^\dagger(\mathbf{x}''')|0\rangle$ and $\hat{\mathcal{C}}_1^\dagger(\mathbf{y})\hat{\mathcal{C}}_2^\dagger(\mathbf{y}')\hat{\mathcal{C}}_3^\dagger(\mathbf{y}'')\hat{\mathcal{C}}_4^\dagger(\mathbf{y}''')|0\rangle$ in subspace $V_0(n)$ are connected by an appropriate number M of fermion hoppings.

To such a Hermitian matrix, we are able to apply the well-known Perron-Fröbenius theorem.[16] It tells us that *the expansion coefficients in Eq. (2) have the same sign and hence ψ_0 is nondegenerate in subspace $V_0(n)$*. To show that it is globally nondegenerate, we need to determine its quantum numbers by the continuity argument. Adiabetically turning off the interactions of Hamiltonian (1), we reduce it to a tight-binding H_0, whose ground state in $V_0(n)$ is a spin-orbital singlet. It implies that ψ_0 is also a spin-orbital singlet and hence is globally nondegenerate.

Next we study the nature of excitations for the case of $N=4n$ with n odd, focusing on whether they are gapless. Following Refs. 3 and 7, we consider the state

$$|\psi_P\rangle = \exp\left[-i\frac{2\pi}{L}\sum_{x=1}^{L} xP(x)\right]|\psi_0\rangle \equiv \hat{O}(P)|\psi_0\rangle, \qquad (3)$$

where operator $P(x)=\Sigma_\alpha v_\alpha n_\alpha(x)$, and the coefficients v_α are to be chosen by the reasoning below. Our aim is to prove gaplessness. In order to do so, we want $|\psi_P\rangle$ to be orthogonal to $|\psi_0\rangle$ and to have an energy expectation value which equals the ground-state energy in the limit $L\to\infty$. The operator $\hat{O}(P)$ "boosts" the crystal momentum of each α component particle by $2\pi v_\alpha/L$. In order to preserve periodic boundary condition, v_α has to be an integer. The state $|\psi_P\rangle$ then has a crystal momentum of $K=(2\pi/L)\Sigma_{x=1}^{L}P(x)$ relative to that of the ground state. Since the Hamiltonian is translationally invariant, and the ground state is nondegenerate, it has a definite crystal momentum. Thus a sufficient condition for the orthogonality condition is $K\neq 2m\pi$, where m is any integer, i.e., K should not be a reciprocal-lattice vector. The expectation energy of $|\psi_P\rangle$ is given by

$$E_P = \langle\psi_P|H|\psi_P\rangle = \langle\psi_0|H'|\psi_0\rangle,$$

where

$$H' = \hat{O}^\dagger H\hat{O}.$$

Since the interacting part of H commutes with $\hat{O}$ the only difference between H' and H is in the tight-binding part, and is given by a phase rotation of each $c_\alpha(x)\to e^{-i2\pi v_\alpha x/L}c_\alpha(x)$. This results in a change of the tight-binding amplitude

$$t \to t_{x,x+1}^{(\alpha)} = te^{-i2\pi v_\alpha/L}, \quad x\neq L$$

and $t_{L,1}^{(\alpha)}=te^{i2\pi v_\alpha(L-1)/L}$. Because v_α is chosen to be an integer, the periodic boundary condition is preserved, and this last bond will remain equivalent to all the other bonds. As a result, the difference $H'-H$ will vanish as $L\to\infty$. More precisely, using $P(x)=n_1(x)$ as an example, we have

$$E_P - E_0 = -t(e^{-i2\pi/L}-1)\sum_x \langle c_1^\dagger(x)c_1(x+1)\rangle + \text{c.c.}$$
$$= -2t\left(\cos\frac{2\pi}{L}-1\right)\sum_x \langle c_1^\dagger(x)c_1(x+1)\rangle,$$

where the last line follows from $\langle c_1^\dagger(x)c_1(x+1)\rangle$ being real for a nondegenerate ground state. Actually, this method can only tell us that there is at least one low-lying state with energy at most of order $1/L$ higher than the ground state. Thus the "gaplessness" may be due to having true gapless excitations or a discrete number of symmetry-breaking states which are degenerate in the thermodynamic limit.[4,17,18] For this reason, our results below should all be taken implicitly as assuming there is no discrete symmetry breaking such as lattice translation.

In particular we consider states generated by the following four operators:

$$P_1(x) = n_1(x),$$

$$P_2(x) = n_1(x) + n_2(x),$$

$$P_3(x) = n_1(x) + n_2(x) + n_3(x),$$

$$P_4(x) = n_1(x) + n_2(x) + n_3(x) + n_4(x). \qquad (4)$$

For general band filling, the crystal momentum K for all four states will not be equal to a reciprocal-lattice vector, they are all orthogonal to the ground state, and there are gapless excitations at K_i generated by P_i. Band fillings equal to $1/4$ $(N=L)$, $1/2$ $(N=2L)$, and $3/4$ $(N=3L)$, however, must be discussed separately.

(i) $1/4$-filled case: the ground state is a SU(4) singlet and we have $N_1=N_2=N_3=N_4=N/4=L/4$, where $N_a=\Sigma_x n_a(x)$. The crystal momenta of the four states given by Eq. (4) are then $\pi/2$, π, $3\pi/2$, and 2π, respectively. Thus all four states are mutually orthogonal to each other, with the first three also orthogonal to the ground state. The fourth state cannot be concluded to be orthogonal to the ground state. Note that except for the noninteracting limit, the crystal momentum for each flavor is not a conserved quantity, only the total crystal momentum. Therefore other combinations like $2n_1$, for example, cannot be shown to be orthogonal to n_1+n_2.

Our analysis establishes that at least at momenta $\pi/2$, π, $3\pi/2\equiv-\pi/2$, there exists gapless excitations. In the large U

limit, where the four-component Hubbard model is mapped into an SU(4) symmetric Heisenberg model, it is known exactly that there are gapless excitations at $K=0$, $\pi/2$, π, and $3\pi/2$ and nowhere else. While our modified LMS approach cannot say anything about $K=0$ and cannot rule out gapless excitations at other K, it supports that the gapless modes are pinned at these K values for all U.

(ii) 3/4-filled case: this case is equivalent to the 1/4-filled case by particle-hole symmetry.

(iii) 1/2-filled case: the ground state is again a singlet and we have $N_1=N_2=N_3=N_4=N/4=L/2$. The four states from Eq. (4) now have momenta $K=\pi$, 2π, 3π, and 4π. Thus we can establish that gapless excitations must exist at $K=\pi$.

While gapless excitations are conclusively shown by the above analysis, they do not tell us much about the excitations beyond the crystal momentum. To try to understand these excitations more, we first consider the single band Hubbard model. By similar approach, one can show that twisted wave functions, for both spin up and down,

$$|\psi_{n_\sigma}\rangle = \exp\left[-i\frac{2\pi}{L}\sum_{x=1}^{L} x n_\sigma(x)\right]|\psi_0\rangle, \qquad (5)$$

have crystal momentum $K=\pi$ at 1/2 filling and are orthogonal to the ground state. In the noninteracting limit, crystal momentum for each spin is conserved, and $\langle\psi_{n_\uparrow}|\psi_{n_\downarrow}\rangle=0$, so there are two distinct gapless modes. In this limit, the gapless excitation with $K=\pi$ is a single particle-hole excitation of $2k_F$ for one of the spins. These can then be cast in spin symmetric combination and spin antisymmetric combinations to give gapless charge and spin excitations. For nonzero U, the Hubbard model at 1/2 filling always has a charge gap and only spin excitations are gapless. Correspondingly, only total crystal momentum is conserved and $|\psi_{n_\uparrow}\rangle$ and $|\psi_{n_\downarrow}\rangle$ no longer have to be orthogonal. Indeed, their overlap $\langle\psi_{n_\uparrow}|\psi_{n_\downarrow}\rangle$ is nonzero as verified by numerical calculations. By rewriting

$$n_\uparrow = \frac{1}{2}(n_\uparrow + n_\downarrow) + \frac{1}{2}(n_\uparrow - n_\downarrow) = \frac{1}{2}n + S_z,$$

one has

$$\exp\left[-i\frac{2\pi}{L}\sum_{x=1}^{L} x n_\uparrow(x)\right] = \exp\left[-i\frac{\pi}{L}\sum_{x=1}^{L} x n(x)\right] \times \exp\left[-i\frac{2\pi}{L}\sum_{x=1}^{L} x S_z(x)\right] = \hat{O}(n)\hat{O}(S_z).$$

In the strong interaction limit, $U\to\infty$, each site tends to be singly occupied, $n(x)\to 1$, so what left is the spin fluctuation $S_z(x)$. For finite U, it would seem that n_1 generates both charge and spin excitations. However, in order for gaplessness, it must be that the overlap with charge excitations must vanish *in the thermodynamics limit*. While we cannot show this rigorously, we can get a partial understanding by considering the single mode approximation state,

$$|\psi_1\rangle = \sum_{x=1}^{L} \exp(i\pi x) n_1(x)|\psi_0\rangle = \frac{1}{2}\tilde{n}(\pi)|\psi_0\rangle + \tilde{S}_z(\pi)|\psi_0\rangle.$$

So $\langle\psi_1|\psi_1\rangle=\frac{1}{4}\langle\tilde{n}(-\pi)\tilde{n}(\pi)\rangle+\langle\tilde{S}_z(-\pi)\tilde{S}_z(\pi)\rangle$. Due to the charge gap, the density-density correlation is finite while the spin-spin correlation diverges as $L\to\infty$. Thus there is no spectral weight for $|\psi_1\rangle$ to be in a charge excitation. Conversely, our proof of gaplessness at π shows that the spin-spin correlation function must diverge at π.

The twisted operator $\exp[-i(2\pi/L)\Sigma_{x=1}^{L} x S_z(x)]$, is what Lieb, Schultz, and Mattis used in their paper (Ref. 3) to show gapless excitation in the Heisenberg model. It cannot be shown to be orthogonal to the ground state in the Hubbard model because it has crystal momentum 0. Instead $n_\sigma(x)$ must be used instead of $S_z(x)$. The fact that $\hat{O}(n_\sigma)$ gives a stronger result than that $\hat{O}(n_\uparrow+n_\downarrow)$ and $\hat{O}(n_\uparrow-n_\downarrow)$ was noted by Yamanaka, Oshikawa, and Affleck.[7]

Returning to the four-component Hubbard model, we discuss the analogous situation for the case of $N=L/4$. In this case, our proof shows gapless excitations for $\pm\pi/2$ and π. In the noninteracting limit, there are four orthogonal choices for P_1 corresponding to whether we use n_1, n_2, n_3, and n_4, and they generate a single particle-hole excitation of $2k_F$. Linear combinations of these can be taken to form charge, spin, orbital, and spin-orbital excitations, the last three corresponding to the three diagonal generators of SU(4). For $U\neq 0$, the four n_α states are not orthogonal, and whether there are three or four gapless modes will depend on whether there is a charge gap (the other three are related by symmetry so they must be all gapless).[13] The "pinning" of gapless excitations at $K=2k_F$ of the noninteracting system was used by Yamanaka, Oshikawa, and Affleck[7] as a generalized definition of Luttinger's Theorem in one dimension. In analogy to the two-component Hubbard model, the gaplessness implies the spin-spin correlation function, the orbital-orbital correlation functions, and the spin-orbital–spin-orbital correlation functions must diverge at $K=\pi/2$. In the strong-coupling limit, charge fluctuations are frozen, and we are definitely left with three gapless excitations, which are the three states with $N_1=N_2=N_3=N_4=N/4$ in the 15 representation of SU(4). For $K=\pi=4k_F$, the gapless excitations for the noninteracting systems are pairs of $2k_F$ particle-hole excitations. The correlation functions that diverge at $4k_F$ are those corresponding to four-particle Green's functions.

For filling factor $N_\alpha=p/q$, with p and q integers, the orthogonality condition that $K\neq 2m\pi$ will be satisfied for $\Sigma_\alpha v_\alpha=1,2,\ldots,q-1$. Accordingly there will be at least q momenta of gapless excitations. In the noninteracting limit, the $\Sigma_\alpha v_\alpha=r$ gapless excitations are r particle-hole pairs. If we assume no broken translational invariance due to interactions (which should be the case for the Hubbard model with only on-site repulsion), then gapless excitations at these momenta persist when $U\neq 0$.[7]

In summary, we studied properties of the ground state and excitations of the four-component Hubbard model, in which electrons carry spin as well as orbital degrees of freedom. Considering cases where total number of electrons $N=4n$

with n odd for periodic boundary condition, we showed rigorously that the ground state of this system is nondegenerate. Using the twist operators as specified in Eq. (4), we addressed the issue of the existence of gapless excitations. We showed that away from the filling factor $1/4$, $1/2$, and $3/4$, the state produced by acting the twist operators [e.g., Eq. (4)] on the nondegenerate ground state is orthogonal to the ground state and its variational energy approaches to the ground-state energy in the thermodynamic limit. For the filling factor equal to $1/4$ and $3/4$, we showed that gapless excitations exist at crystal momenta $\pi/2$, π, $3\pi/2 \equiv -\pi/2$.

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[1] Y. Tokura and N. Nagaosa, Science **288**, 462 (2000).
[2] Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. Lett. **81**, 3527 (1998); Phys. Rev. B **60**, 12 781 (1999).
[3] E. H. Lieb, T. D. Schulz, and D. C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[4] I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
[5] Y. Q. Li, Phys. Rev. Lett. **87**, 127208 (2001).
[6] E. H. Lieb, Phys. Rev. Lett. **62**, 1209 (1989).
[7] M. Yamanaka, M. Oshikawa, and I. Affleck, Phys. Rev. Lett. **79**, 1110 (1997).
[8] S. Pati, R. Singh, and D. I. Khomskii, Phys. Rev. Lett. **81**, 5406 (1998).
[9] B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[10] Y. Yamashita, N. Shibata, and K. Ueda, Phys. Rev. B **58**, 9114 (1998).
[11] Y. Yamashita, N. Shibata, and K. Ueda, J. Phys. Soc. Jpn. **69**, 242 (2000).
[12] C. Itoi, S. Qin, and I. Affleck, Phys. Rev. B **61**, 6747 (2000).
[13] P. Azaria, A. O. Gogolin, P. Lecheminant, and A. A. Nersesyan, Phys. Rev. Lett. **83**, 624 (1999); P. Azaria, E. Boulet, and P. Lecheminant, Phys. Rev. B **61**, 12 112 (2000).
[14] E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).
[15] G. S. Tian and H. Q. Lin, Phys. Rev. B **67**, 245105 (2003).
[16] J. Franklin, *Matrix Theory* (Prentice-Hall, Englewood Cliffs, NJ, 1968).
[17] M. Ma, G. S. Tian, and H. Q. Lin (unpublished).
[18] E. H. Lieb and D. C. Mattis, J. Math. Phys. **3**, 749 (1962).