Degeneracy of Ground State in Two-dimensional Electron-Lattice System

Tetsuya Hamano and Yoshiyuki Ono

Department of Physics, Toho University, Miyama 2-2-1, Funabashi, Chiba 274-8510

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In a recent paper\(^1\) we have reported the ground state of a two dimensional system described by a SSH(Su-Schrieffer and Heeger)-type Hamiltonian with a half-filled electronic band. The Hamiltonian\(^2\) is given by

\[
H = -\sum_{i,j,\sigma} \left[ (1 - x_{i,j})(C_{i,j,\sigma}^\dagger C_{i+1,j,\sigma} + \text{h.c.}) + (1 - y_{i,j})(C_{i,j,\sigma}^\dagger C_{i,j+1,\sigma} + \text{h.c.}) \right] + \frac{1}{2\lambda} \sum_{i,j} \left[ a_{i,j}^2 + y_{i,j}^2 \right],
\]

(1)

where the field operators \(C_{i,j,\sigma}\) and \(C_{i,j,\sigma}^\dagger\) annihilate and create an electron with spin \(\sigma\) at the site \((i, j)\) on a square lattice subject to the periodic boundary conditions (PBC), and the energy is scaled by the transfer integral of the regular lattice, the bond variables \(x_{i,j}\)’s and \(y_{i,j}\)’s in \(x\)- and \(y\)-directions, respectively, being scaled appropriately to involve the electron-lattice coupling coefficient, \(\lambda\) representing the dimensionless coupling constant. In present work we fix the coupling constant at \(\lambda = 0.3\), because we are interested only in the properties of the ground state which would not depend on the value of \(\lambda\). The ground state is accompanied by lattice distortions which have Fourier components not only with the nesting vector \(Q = (\pi/a, \pi/a)\) but also with many other wave vectors parallel to \(Q\).\(^3\)

\[
x_{i,j} = x_{i,j}^N + x_{i,j}^O, \quad y_{i,j} = y_{i,j}^N + y_{i,j}^O,
\]

(2) \(\quad\)

(3) \(\quad\)

\[
x_{i,j}^N = X_{\frac{i}{a}, \frac{j}{a}} (-1)^{i+j},
\]

\[
x_{i,j}^O = \sum_{0 < q < \pi/a} (X_{q,q} e^{i(q+j)a} + X_{q,q}^* e^{-i(q+j)a}),
\]

(4)

and a similar expression for \(y_{i,j}\). Here \(a\) represents the lattice constant. Furthermore, the pattern of these distortions is found not unique in the lowest energy state, although the structure of the electronic energy spectrum and the total energy of the system are the same.\(^4\) In this note we discuss the degrees of degeneracy of the lowest energy state for the model described by eq. (1).

It is clear that there is trivial degeneracies due to the symmetry of the system. Three examples of the distortion patterns in the ground state is shown in terms of the wave number dependence of the Fourier components. In each graph, the amplitudes of \(X_{q,q}\) and \(Y_{q,q}\) are plotted as functions of \(q\) (\(0 < q \leq \pi/a\)) on the left-hand side, while their arguments are shown on the right-hand side. The amplitudes are exactly the same in (a) and (b) of Fig. 1 though the arguments look quite different. It is not difficult to understand that the difference between Figs. 1(a) and 1(b) can be explained by the translation symmetry of the system. The behavior of the amplitudes in Fig. 1 (c) is completely different from that in Figs. 1(a) and 1(b). This fact indicates that there exist non-trivial degeneracy in the ground state. From Fig. 1 along with many other data which are not shown here, we can summarize the characteristics of the distortion patterns in the ground state as follows; (1) the amplitude of \(X_{q,q}\) is always equal to that of \(Y_{q,q}\), (2) the argument of \(X_{q,q}\) is equal to that of \(Y_{q,q}\) or differs from that of \(Y_{q,q}\) by \(\pi\), and (3) the values of \(X_{\frac{\pi}{a}, \frac{\pi}{a}}\) and \(Y_{\frac{\pi}{a}, \frac{\pi}{a}}\) are common for all the patterns. Thus the variety of the distortion patterns in the ground state can be said to be determined by the

Fig. 1. The wave number dependence of the Fourier components of the lattice distortion. The system size is \(32 \times 32\). For the definition of \(X_{q,q}\) and \(Y_{q,q}\), see eqs. (2) to (4).
values of $X_{q,q}$’s with $0 < q < \pi/a$.

In order to discuss the degrees of degeneracy of the ground state, we assume first that the Fourier components of the distortion are restricted to the diagonal ones with $q_x = q_y$ as numerically confirmed in the previous paper[6] and that the displacements $y_{i,j}$ in $y$-direction are automatically determined if the displacements $x_{i,j}$ in $x$-direction are fixed. Then the number of variable describing the distortion pattern can be reduced from $2 \times (N - 1)^2$ to $N - 1$ for a system with the size $N \times N$. It will be allowed to choose $x_{i,j}$ ($i = 1, 2, \cdots, N - 1$) with a fixed $J$ as a set of $N - 1$ independent variables. (Note the constriction $\sum_i x_{i,j} = 0$ due to the PBC.)

\begin{figure}[h]
\centering
\includegraphics{fig2.png}
\caption{$x_{i,j}^O$ for a fixed $J$ is plotted as a function of $i$. (a), (b) and (c) correspond to those of Fig. 1. The value of $J$ is taken to be 1 in these cases. Changing $J$ leads to a translation of the pattern in the direction of $x$ (or $i$).}
\end{figure}

Figures 2(a) to 2(c) show the distortion $x_{i,j}^O$ for a fixed $J(=1)$ as a function of $i$, which is constructed from $X_{q,q}$’s with $0 < q < \pi/a$ of the corresponding figures of Fig. 1 as in eq. (4). It will be clear that Figs. 2(a) and 2(b) can be completely overlapped by a simple translation along $i$-axis. On the other hand Fig. 2(c) is quite different from them. Nevertheless there exists a common feature among the three patterns. Namely, (I) $x_{i,j}^O$ vanishes at every second site, and (II) the number of sites at which it is positive is the same as the number of sites with negative value. Furthermore (III) the absolute values of the positive and negative $x_{i,j}^O$’s are equal to each other and common to all the three patterns. It will be plausible to assume that the absolute value is determined by the dimensionless coupling constant $\lambda$. All the numerical data we have obtained show that there is no rule in the order of positive and negative $x_{i,j}^O$’s. Thus we can conjecture that the degeneracy of the ground state is given by different order of positive and negative $x_{i,j}^O$’s. If $N$ is a multiple of four, then $x_{i,j}^O$ will be zero at a half of $N$ sites ($i = 1, \cdots, N$) and will be positive at a half of remaining $N/2$ sites and negative at remaining $N/4$ sites.

The degree of non-trivial degeneracy except the trivial degeneracy due to arrangement of zero points might be said to be $N^2 C_{N/4}$ ($\simeq N^{N/4}$ for $N \gg 1$).

In order to check whether the above-mentioned rule, (I) to (III), for the distortion pattern is a sufficient condition for the ground state, we calculate, for the system size $32 \times 32$, the total energy for all the lattice distortion patterns satisfying the above-mentioned rule, whose number is $16 C_8 = 12,870$. For the amplitude of nonvanishing $x_{i,j}^O$, we use the value shown in Fig. 2. In all the cases the resulting energy is found equal to the minimum energy. Thus the above-mentioned rule can be regarded as a sufficient condition.

It is not easy to show the above rule is a necessary condition for the ground state distortion pattern. However we can confirm it numerically to some extent. As discussed in the previous paper[6] we may believe that the ground state distortion for the present model has only the Fourier components with $q_x = q_y$. In this situation we can reduce the 2D Schrödinger equation to a 1D equation in the momentum space[1]. In order to perform the calculations finding the ground state effectively, we adopt this formulation. We start the iterative calculation by giving random numbers for the diagonal Fourier components of the distortions $x_{i,j}$’s and $y_{i,j}$’s and continue the iteration up to the 100-th step. The number of runs carried out is 100,000. Out of all the runs we could obtain 20,445 minimum energy states[2] some of them are equivalent within the translational shift. We could confirm that the above rule is satisfied by all the lowest energy states obtained in these calculations. Since we find no counter example against the above rule in a number of calculations starting from random initial inputs, it may be allowed to say that the above-mentioned rule is a necessary condition for the ground state distortion pattern of the present model. We have confirmed the above rules for different system sizes, $N = 8, 12, 16, 32, 64$ and 128, though the sample number for $N = 64$ and 128 are rather restricted, and also for tilted square systems satisfying PBC’s.

The degeneracy treated in this paper is considered to be due to the highly symmetric structure of the model. The Peierls distortions in two-dimensional anisotropic systems are now under investigation. The results will be published elsewhere.

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[2] W. P. Su, J. R. Schrieffer and A. J. Heeger: Phys. Rev. B 22 (1980) 2099.
[3] If we increase $J$ by one, the pattern shifts to larger $i$ direction by one.
[4] Since there are other local minima, it is not possible to get the lowest energy state in all of the runs. A typical local minimum is the one studied by Tang and Hirsch (Phys. Rev. B 37 (1988) 9546), which has only the Fourier component with the nesting wave vector.
[5] E. Dagotto: Rev. Mod. Phys. 66 (1994) 763.