Phases and Density of States
in a Generalized Su-Schrieffer-Heeger Model

Khee-Kyun Voo\textsuperscript{a,b}, Chung-Yu Mou\textsuperscript{b,c}

\textsuperscript{a}Texas Center for Superconductivity at the University of Houston, Houston, TX 77204, USA
\textsuperscript{b}Department of Physics, National Tsing-Hua University, Hsinchu 30043, Taiwan
\textsuperscript{c}National Center for Theoretical Sciences, P.O.Box 2-131, Hsinchu, Taiwan

Abstract

Self-consistent solutions to a generalized Su-Schrieffer-Heeger model on a 2-dimensional square lattice are investigated. Away from half-filling, spatially inhomogeneous phases are found. Those phases may have topological structures on the flux order, large unit cell bond order, localized bipolarons, or they are simply short-range ordered and glassy. They have an universal feature of always possessing a gap at the Fermi level.

Key words: SSH model, topological structure, gapped Fermi level
PACS: 63.20.Kr, 71.10.Fd, 71.23.An, 71.38.Ht, 71.38.Mx, 71.45.Lr

The Su-Schrieffer-Heeger (SSH) model \cite{Heeger1} was motivated by the quasi-1-dimensional conducting polymer polyacetylene. The model exhibits Peierls instability at the characteristic wavevector $2k_F$, where $k_F$ is the Fermi wavevector that depends on the band filling. As a result the translational symmetry of the lattice is spontaneously broken and a gap is opened up at the Fermi level of the electronic spectrum. Since the lattice distortion in the ground state is multiply degenerated, topological mid-gap soliton states can be formed at the domain boundaries. In-gap polaron states can also be formed as soliton-antisoliton bound states. At the empty band limit, bipolaron states are favored. The above mentioned states as the elementary excitations of the system and their experimental consequences were reviewed in detail in an article by Heeger \textit{et al.} \cite{Heeger1} In dimensions higher than one, for instance in a 2-leg ladder, a new mid-gap soliton named the “twiston” was discovered \cite{Kimura}. The ground state in the half-filled 2-dimensional (2D) square lattice was also studied within an assumption of a small unit cell \cite{Lazarides, Chang, Chang2}, or using some more elaborated numerics \cite{Mou}. In general, studies of the model in higher dimensions are relatively fewer,
and knowledge of the possible phases is limited. Therefore investigations of the phases in some higher dimensional SSH-type models are desirable. In this paper, we have extended these studies to a generalized SSH model in two dimension (2D). It is found that generally speaking, the types of phase are much more diverse in 2D. Some of them appear to be nice generalizations of the above-mentioned states in one dimension (1D). In particular, the translational symmetry is also spontaneously broken and the Fermi levels are gapped in many phases. Thus this generalized SSH model represents an insightful generalization of the conventional model and merits serious consideration.

We start by considering the conventional SSH model in the adiabatic limit,

\[
H_{\text{SSH}} = -\sum_{i,\sigma} \sum_{n=\pm x, \pm y} (t + \alpha \phi_{i+n,i}) c_{i\sigma}^{\dagger} c_{i+n,\sigma} + \frac{\kappa}{2} \sum_{i,\sigma} \sum_{n=\pm x, \pm y} |\phi_{i,i+n}|^2, \tag{1}
\]

where \( t \) is the hopping, \( \alpha \) is the electron-lattice coupling, \( \kappa \) is the interatomic elastic constant, and \( \phi_{j} \equiv a - |r_i - r_j| \) is the deviation of an interatomic distance from its equilibrium value \( a \). Every quantity here is real-valued and \( \alpha \) and \( \kappa \) are positive. To find the zero temperature configuration of the lattice, \( \phi_{i+n,i} \)'s are treated as variational parameters and adjusted (through some procedures such as the steepest-descent method) to minimize the total energy \( \langle H_{\text{SSH}} \rangle \). Alternatively, one can recast the minimization problem into an equivalent self-consistency problem using \( \partial \langle H_{\text{SSH}} \rangle / \partial \phi_{ij} = 0 \), which leads to \( \phi_{ij} = (2\alpha/\kappa) \sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} > \) and \( \phi_{i+n,i} \) is now a bond parameter to be solved by numerical iteration. Defining \( \Phi_{ij} = \alpha \phi_{ij} \) and \( \lambda = 4\alpha^2/\kappa \), the problem is reformulated as

\[
H_{\text{SSH}} = -\sum_{i,\sigma} \sum_{n=\pm x, \pm y} (t + \Phi_{i+n,i}) c_{i\sigma}^{\dagger} c_{i+n,\sigma} + \frac{\lambda}{2} \sum_{i,\sigma} \sum_{n=\pm x, \pm y} |\Phi_{i,i+n}|^2, \tag{2}
\]

\[
\Phi_{ij} = \frac{\lambda}{2} \sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} >. \tag{3}
\]

In this form, it is easy to see that the only quantity characterizing the problem is \( t/\lambda \) or \( \kappa t/(4\alpha^2) \), which is dimensionless.

In the formulation Eq. 2 and 3, it will be meaningful to extend \( \Phi_{ij} \) from the real number regime into the complex number regime. The physical appeal of the extension is that the model now addresses a class of more general problems by the following reason. Generally, the parameter \( \Phi_{ij} \) represents an overlap integral \( <\psi_i|H'|\psi_j> \) describing off-site electronic correlations, with \( H' \) and
Fig. 1. The 2-sublattice ansatz. The 2D square lattice is patched up by centering this cross at sites belong to one of the two sublattices. The complex-valued nature is indicated by an arrow, which means that $\Phi_{ij}^{2SL} = \Phi_{ji}^{2SL}$ is the reversed arrow and may not be identical to $\Phi_{ij}^{2SL}$.

$|\psi_{ij}\rangle$ being the off-site part of the total Hamiltonian and the local atomic wavefunctions respectively. Since in addition to the electron-lattice interaction, a renormalized low-energy effective theory may contain other many-particle effects manifested in the overlap integral, there is no reason for $\Phi_{ij}$ to be necessarily real when these effects are included. This extension thus goes beyond the electron-lattice interaction and it may be viewed as a prototype of this class of problems. Indeed, a four-fermion interaction is generated at integrating out $\Phi_{ij}$, and therefore the self-consistency equation that $\Phi_{ij}$ respects can also be regarded as a mean field equation. In fact, the model is formally the same as a mean field theory in the high-$T_c$ cuprates [7]. In view of this connection, we have in this paper investigated this generalized SSH model in detail. On one hand, our study is a generalization of the conventional SSH model in 2D; on the other hand, it is also a study complementary to those mean field studies of the high-$T_c$ system, where a different parameter regime (larger $t/\lambda$) was emphasized.

It is noted that the generalized hamiltonian bears the same form as a mean field hamiltonian in the high-$T_c$ cuprates [7], and presumably they should bear the same solution. In the high-$T_c$ context, a 2-sublattice (2SL) ansatz
(see Fig. 1) designed to capture any \((\pi, \pi)\)-instability was adopted in Ref. [7] for the solution. Such a high translational symmetry solution might be appropriate in that context, since other effects such as fluctuation might at work and preserve the symmetry to a high degree, but in our case, where we expect soliton or polaron solutions, such an ansatz at the outset is clearly inappropriate. Nevertheless, we still have reproduced the solution within that framework and compare with the result of our approach which allows spatially nonhomogeneous solutions. The 2SL ansatz assumes the distribution of \(\Phi\)'s on the lattice has a repeating unit as shown in Fig. 1. Different types of solution are also solved and compared with the result of our unrestricted search. Our unrestricted-bond iteration converges to the 2SL form only at two regimes, (i) \(x \sim 0\) and \(t > t_c \sim 0.1\alpha\), where the uniform-SF is located at; and (ii) large \(t\) and \(x\), where the uniform real-bond phase is located at. \(x\) is the hole concentration between 0 and 1.

Away from the above regimes, our solutions generally do not fit in a 2SL ansatz. Some representative phases which we will discuss and their energies (per site) \(E_G\) are grouped here beforehand. In the brackets, energies \(E_G^{2SL}\) and phases from the 2SL ansatz are also given for comparison. We obtain dimer-box (D-B) glass phase at, \(t = 0, x = 0.3\), with \(E_G = -0.1750\lambda\ [E_G^{2SL} = -0.1608\lambda, \ K]\); \(t = 0, x = 0.5\), with \(E_G = -0.1250\lambda\ [E_G^{2SL} = -0.1077\lambda, \ u-R]\). We find striped-staggered-flux (s-SF) at, \(t/\lambda = 0.2, x = 0.1\), with \(E_G = -0.5017\lambda\ [E_G^{2SL} = -0.4991\lambda, \ u-SF]\); \(t/\lambda = 0.2, x = 0.2\), with \(E_G = -0.4784\lambda\ [E_G^{2SL} = -0.4733\lambda, \ u-R]\); \(t/\lambda = 0.4, x = 0.1\), with \(E_G = -0.8134\lambda\ [E_G^{2SL} = -0.8088\lambda, \ u-SF]\). Wigner lattice of bipolarons (WBP) is found at, \(t/\lambda = 0.1, x = 0.75\), with \(E_G = -0.1267\lambda\ [E_G^{2SL} = -0.1232\lambda, \ u-R]\). A bond order wave (BOW) which we have named Real-staggered-box (RSB) is found at, \(t/\lambda = 0.1, x = 0.5\), with \(E_G = -0.2402\lambda\ [E_G^{2SL} = -0.2390\lambda, \ u-R]\); \(t/\lambda = 0.05, x = 0.5\) with \(E_G = -0.1798\lambda\ [E_G^{2SL} = -0.1734\lambda, \ u-R]\). Solutions of lower translational symmetry, when they exist, are found to have lower energies and the percentage of difference is more prominent at small \(t\) but intermediate \(x\). Typical total density of states (DOS) of these phases are shown in Fig. 2.

**Dimer-box glass:** On the \(t = 0\) axis, a solution of high degeneracy can be found analytically. It is straightforward to verify that a lattice *arbitrarily* filled with disjointed dimers and boxes is a solution [13]. A dimer [7,12] is
Fig. 2. Total density of states at some representative dopings and hoppings ($\lambda = 1$): The shaded are occupied levels and the horizontal axis of each box is the energy from $-2.5$ to $+2.5$.

a doubly filled nearest-neighbor bond [19] with $|\Phi| = \lambda/2$. A box [14] is a plaquette with bonds

$$|\Phi_{12}| = |\Phi_{34}|, \quad |\Phi_{23}| = |\Phi_{41}|,$$

$$|\Phi_{12}|^2 + |\Phi_{23}|^2 = \left(\frac{\lambda}{2}\right)^2,$$

and a real

$$\Phi_{12}\Phi_{23}\Phi_{34}\Phi_{41} < 0,$$

where 1, 2, 3, and 4 are consecutive corners of the plaquette. The lowest two levels of a box are filled with 4 electrons. Both dimer and box have an average of 1 electron per site, energy $-\lambda/4$ per site, and only two levels at $\pm \lambda/2$. At $x = 0$, the lattice is fully filled with dimers and boxes. At $x > 0$, a solution can be simply obtained by plucking off dimers or boxes [15] from the lattice and the energy will be just $-(1-x)\lambda/4$. Creating empty sites also creates zero energy states, therefore the spectrum of a doped zero-$t$ system is a three-level structured DOS $D(\varepsilon) = x\delta(\varepsilon) + (1-x)[\delta(\varepsilon + \lambda/2) + \delta(\varepsilon - \lambda/2)]$. Since the arrangement of the dimers and boxes is arbitrary, this phase is in general a
glass of bond and plaquette centered electron charges. But it is important to note that due to the degeneracy condition Eq. 5, a box can be continuously deformed into two dimers or vice versa without any energy barrier intervening. Therefore this glass might not be a stable phase when fluctuation effect is taken into account, and some translational symmetry is expected to be restored.

It can be shown analytically that the D-B glass has a lower energy than the u-R phase at $t = 0$ and $x \to 1$. At $x \to 1$, the kinetic energy of a u-R phase is simply obtained by filling in the band bottom, i.e., $-2D(t + \Phi)(1 - x)$, and the potential energy is $2D\Phi^2/\lambda$, where $D = 2$ is the dimensionality. Minimizing the total energy gives $\Phi = (1 - x)\lambda/2$, hence energy $E_G^{2SL} = -2tD(1 - x) - (\lambda D/2)(1 - x)^2$. It is of $\mathcal{O}[(1 - x)^2]$ at $t = 0$, while the D-B glass has $E_G = -(1 - x)\lambda/4$ of $\mathcal{O}[(1 - x)]$. Comparing $E_G^{2SL}$ and $E_G$ also gives a scale $t = \lambda/(8D)$ at which the D-B glass is destabilized and there is a crossover from short-range-order (SRO) to long-range-order (LRO).

At intermediate $x$, one can only obtain $E_G^{2SL}$ numerically. We have studied, e.g., $x = 0.1, 0.3$, and 0.5, and have found that they have energies (which are given before, and are stable at lattices $40 \times 40, 80 \times 80$, and $120 \times 120$) substantially higher than the D-B glass. A feature to note is that the 2SL phases are ungapped, whereas the three-level D-B glass is obviously gapped. The levels expand into bands at small but nonzero $t$ and the gapping remains, as a vestige of the zero-$t$ phase.

**Striped-staggered-flux:** At the regime $0 \lesssim x \lesssim 0.2$ and $t_c(\sim 0.1\lambda) < t \lesssim 0.6\lambda$, the holes are found to arrange into stripes along the lattice axes [16,17] (say $y$-axis, see Fig. 3). Whereas uniform-SF is obtained within the 2SL ansatz. The stripes at the meantime are also topological domain walls separating antiphase SF domains [17]. Two types of domain walls are found, one has a column of neutral-flux plaquettes inserted, the other has a column of plaquettes deleted. It is remarkable that the electron depletion can be as large as $\sim 0.2$ and has a short coherence length of only a few lattice constants. We also make an observation that it has one hole per unit length [18]. The spectrum [see Fig. 2(b), (e), and (f)] is nodally gapped at the Fermi level and the gap maxima at $(0, \pm \pi)$ and $(\pm \pi, 0)$ [7,12,8,9,10,11] manifest themselves as the van Hove singularity peaks in the DOS. Local DOS shows that the mid-band has a great part composed of states localized along the stripes (see Fig. 3).

It is interesting to check if such striped-SF phase have energies lower than that of the 2SL phases. For some commensurate fillings like $x = 0.1, 0.2$, and 0.3, we have obtained straight hole-stripes along one of the lattice axes. In such cases, the fact that the striped-SF phase have lower energy can be justified in the thermodynamic limit as follows. Owing to the translational invariance along one axis, we may equivalently seek for such solution within an ansatz with translational symmetry $\Phi_{i,1+\hat{a}} = \Phi_{i+2\hat{g},1+\hat{a}+2\hat{g}}, \hat{a} = \hat{x}, \hat{y}$ [20].
Fig. 3. Topological stripe: (Top) The bond current \((4t/\lambda)\text{Im}\Phi_{ij}\), orbital moment (average of directed bond currents round a plaquette), and (middle) electron density profiles across an 1D antiphase domain wall \((t/\lambda = 0.2, x = 0.1)\). Bond thicknesses are proportional to the current sizes and circle areas to the moment sizes. Maximum bond current here is 0.106/s, and maximum moment is 0.105/s. The domain wall shown here contains neutral plaquettes. (Bottom) Typical local DOS at hole-rich and hole-poor sites are also shown.

Due to the reduction of numerical effort (diagonalizing a hamiltonian on a \(N_x \times N_y\) lattice is now separately diagonalizing \(N_y/2\) hamiltonians on \(N_x \times 2\) lattices), self-consistent solutions can now be pursued on much larger lattices. We have justified that the striped-SF at, e.g., \(t/\lambda = 0.2, x = 0.1, 0.2\), and \(t/\lambda = 0.4, x = 0.1\) have energies (which are given before) lower than that of the 2SL solutions. The energies are stable at lattices from 40\(\times\)40 to 120\(\times\)120.

Note that the stripes here are not a result of frustrated phase separation since we assume no repulsion between holes. They are more appropriately understood as soliton states created to accommodate the holes, analogous to the soliton states in the 1D SSH model [1]. By segregating out the holes, the SF order has survived into higher hole concentrations where it would not have existed within the 2SL ansatz.

**LRO-SRO crossover:** The nonzero but small \(t\) regime, \(t < t_c \sim 0.1\lambda\) is a crossover region between the large-\(t\) regime of LRO and the zero-\(t\) regime of degenerated glass. SRO dominates over this regime and there are lots of almost-degenerate local minimum solution. Phases in this regime are generally glassy, have complex bonds at \(x < 0.3\), and real bonds at \(x > 0.3\). Charge distribution is correlated with the local bond order and also nonuniform in
Fig. 4. (Left) Real-staggered-box BOW with uniform charge distribution at \( t/\lambda = 0.1, x = 0.5 \). (Right) Wigner lattice of bipolarons at \( t/\lambda = 0.1, x = 0.75 \). Bond thicknesses and circle areas are drawn proportional to the bond magnitudes and electron densities respectively.

In general, regions that are crowded with electrons may have complex bonds and regions that are not, have essentially real bonds. In our calculation, such glassy states found by iteration do have energies lower than that of the 2SL solution and their spectra are always gapped at the Fermi level.

At \( x \sim 1 \) of this crossover regime, the obtained state contains uncorrelated scattered bipolarons. A bipolaron is a localized state occupied by two electrons, with nonzero real bonds at its vicinity. Decreasing \( t \) shrinks them into dimers, or increasing electron density turns them into an almost-hexagonal closed-packed Wigner lattice (WBP) (see Fig. 4). In the well-isolated bipolarons regime, the energy can be readily obtained as the sum of the energies of the individual bipolarons. For the Wigner lattice, for instance at \( t/\lambda = 0.1, x = 0.75 \), we obtain the same energy (which is given before) at lattices from 20×20 to 32×32, and it is lower than the energy of the 2SL solution (also given before).

Two exceptions out of these glassy phases are the BOWs with uniform charge distribution named “real-staggered-box” (RSB) (see Fig. 4) found at \( x = 0.5 \), and “box-staggered-flux” (B-SF) at \( x = 0 \). RSB found at \( t/\lambda = 0.1 \) and 0.05 have energies (which are given before, and are stable at lattices from 40×40 to 120×120) lower than that of the u-R. B-SF is a phase with SF order and stronger bonds distributed like a square array of boxes (resembles those boxes in Ref. [7]), and it also has energies lower than that of SP.
Fig. 5. Approximate phase diagram: B-SF: Box-staggered-flux (gapped). u-SF: Uniform staggered-flux (ungapped when \( x > 0 \)). s-SF: Striped-staggered-flux (gapped). u-R: Uniform real-bond (ungapped). D-B: Dimer-Box glass (gapped). The dimer and box order are exact only at \( t = 0 \). g-R: Phases with glassy real-bond and charge density (gapped), and are not characterizable by a simple order. RSB: Real-staggered-box BOW with uniform charge density (gapped). WBP: Wigner lattice of bipolarons (gapped). i-BP: Isolated and uncorrelated bipolarons (gapped).

When \( x < 0.3 \), bonds are complex but remain glassy. The spectrum has a narrow in-gap band consists of almost-localized states. These in-gap states are fundamentally different from those of the striped-SF at larger \( t \). The latter are soliton states supported by the LRO, while the former are states localized in the bond glass.

In summary, an approximate phase diagram is given in Fig. 5. Spatially non-homogeneous phases are shown to be energetically more favorable in the generalized SSH model in 2D away from half-filling, and the electronic spectrum is believed to show a similar gapped Fermi level as that in the 1D conventional SSH model. The doped holes also go into the in-gap states and topological object may also be formed, but the 2D phases are much more complicated than the simple polymerizations in 1D. Those phases may be superstructured or short-range-ordered. At large \( t/\lambda \) and large \( x \), the translational symmetry is preserved and this is fundamentally different from the 1D case, where the Peierls instability always in effect.
We thank the support from the National Science Council of Taiwan under grant no. NSC91-2112-M-007-049, and National Center for Theoretical Sciences (Phys. Div.) of Taiwan for letting us to use their facilities. KKV also thanks the support from the Texas Center for Superconductivity at the University of Houston and a grant from the Robert Welch Foundation.

References

[1] A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W.-P. Su, Rev. Mod. Phys. 60, 781 (1988).
[2] S. Mazumdar, Phys. Rev. B 39, 12324 (1989); 36, 7190 (1987).
[3] S. Tang and J. E. Hirsch, Phys. Rev. B 37, 9546 (1988); 39, 12327 (1989).
[4] Y. Ono and T. Hamano, J. Phys. Soc. Jpn 69, 1769 (2000).
[5] M. T. Figge, M. Mostovoy, and J. Knoester, Phys. Rev. Lett. 86, 4572 (2001).
[6] Q. Yuan and T. Kopp, Phys. Rev. B 65, 85102 (2002).
[7] I. Affleck and J. B. Marston, Phys. Rev. B 37, 3774 (1988); J. B. Marston and I. Affleck, Phys. Rev. B 39, 11538 (1989).
[8] T. C. Hsu, J. B. Marston, and I. Affleck, Phys. Rev. B 43, 2866 (1991).
[9] M. U. Ubbens and P. A. Lee, Phys. Rev. B 46, 8434 (1992).
[10] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B. 63, 094503 (2001).
[11] D. F. Schroeter and S. Doniach Phys. Rev. B 66, 075120 (2002).
[12] T. Dombre and G. Kotliar, Phys. Rev. B 39, 855 (1989).
[13] S. Sachdev, Phys. Rev. B 41, 4502 (1990).

[14] We note that the box order discussed here is a more general case of that discussed in Ref.[7] and [12] which has $|\Phi_{12}| = |\Phi_{23}| = |\Phi_{34}| = |\Phi_{41}|$.

[15] If the number of electron is odd, it is energetically more favorable for the unpaired electron to form a singly filled dimer with $|\Phi| = \lambda/4$ and energy $-\lambda/8$, rather than breaking the bond entirely forming an empty site and a nonbonded electron with energy 0. In the former case the singly filled dimer contains charge 1 and spin 1/2 (“polaron”). In the latter case the empty site contains charge 1 (taking the half-filled site as reference) but spin 0 (“holon”), and the unpaired electron contains spin 1/2 but charge 0 (“spinon”).

[16] Addition of further hoppings such as a next-nearest-neighbor hopping disrupts the orientation of the stripes.
[17] If the hole number in the finite lattices does not support hole-strings long enough to span the periodic lattice, they form smaller closed hole-strings and are still antiphase boundaries of the SF domains.

[18] Analogous antiphase structure defined by staggered-current correlation was also found in a density matrix renormalization group calculation on a rather different model by U. Schollwock et al. (cond-mat/0209444). Holes are also found to accumulate at the boundary with the same density, but their current-current correlation is dynamical whereas ours is static.

[19] The dimers are in fact bipolarons of the smallest size.

[20] This ansatz includes the 2SL ansatz and the box order.