Deconstructing Magic-angle Physics in Twisted Bilayer Graphene with a Two-leg Ladder Model

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We study the single- and many-particle properties of a two-leg ladder model threaded by a flux with the legs coupled by a spatially varying term. Although a priori unrelated to twisted bilayer graphene (TBG), the model is found to have striking similarities: A quasiflat low energy band emerges with characteristics similar to that of magic angle TBG. We study the effect of interparticle interaction in our model using the Density Matrix Renormalization Group and find that when the band is quasiflat, the ground state is a ferromagnetic Mott insulator. As the band becomes more dispersive, the system undergoes a ferromagnetic to antiferromagnetic transition. We discuss how our model is relevant not only to magic-angle physics in TBG, but also in the larger context of 1D correlations and magnetism.

In recent years it has been realized that rotating two graphene layers by a small relative angle away from AA or AB configuration results in unexpected properties. In such systems, dubbed twisted bilayer graphene (TBG), the low-energy bands become quasiflat at an angle of ∼ 1°, called the “magic angle” [1–3]. With kinetic energy suppressed, interactions are effectively enhanced, leading to rich, correlated phases seen in experiments [4–11]. In particular, insulating states that cannot be explained by single particle band theory appear when each of the conduction and valence bands is half-filled. Further, doping away from half-filling gives way to superconducting phases. The phase diagram is reminiscent of that in the cuprates, adding to the excitement, and intense efforts are under way to understand the nature of the ground state.

A major challenge in studying correlation effects in magic angle TBG is that its single-particle physics is not well understood. Rotation between the two layers leads to a large scale moiré pattern and an enlarged supercell which makes ab initio calculations impossible [2]. Long-wavelength descriptions in momentum space, which treat the interlayer coupling perturbatively, exist for general rotations but break down at the magic angle [3]. Attempts to write effective real-space lattice theories by constructing appropriate Wannier functions have revealed that the Wannier functions are not very well localized [12–14]. Thus, a suitable starting point at the single-particle level is lacking, which has resulted in a variety of competing theories for the correlated physics. Alternative approaches that provide clues to the physics of magic-angle TBG are, therefore, needed.

In this Letter, we provide such an approach by defining an auxiliary model which is a priori unrelated to TBG, nevertheless captures aspects of TBG both at the single- and many-particle levels. In particular, we show that a two-leg ladder pierced by a flux with the legs coupled by a spatially varying term leads to a quasiflat low-energy band with characteristics similar to that in magic angle TBG. At half-filling of this band, interactions lead to an insulating state with intra- as well as inter-leg ferromagnetic ordering between spins. As the bandwidth increases, both orders turn antiferromagnetic. We discuss the relevance of our findings in light of recent works on TBG. We also explore how our model is pertinent to the broader context of 1D correlations and magnetism.

At low energies, a TBG can be described by

\[ h_{1,2} = -i \gamma_0 \left( \begin{array}{cc} 0 & \partial_x - i \partial_y \\ 0 & 0 \end{array} \right), \]

\[ h_{\perp} = \gamma_0 \frac{2}{3} \sum_{n=0}^{2} e^{i \delta K_n \cdot r} \left( \begin{array}{cc} 1 & e^{-i \frac{2\pi n}{3}} \\ e^{i \frac{2\pi n}{3}} & 1 \end{array} \right). \]

where \( h_{1,2} \) are Dirac Hamiltonians describing the individual layers and \( h_{\perp} \) describes interlayer coupling. Here, \( \gamma_0 \) is the Dirac velocity of the individual layers, \( \gamma_0 \) is the interlayer coupling strength, \( \delta K = K_\theta - K \) is the vector that connects the Dirac points of the rotated and the unrotated layers in momentum space, and \( \delta K_n \) is \( \delta K \) rotated by an angle of \( 2\pi n/3 \). The vector \( \delta K \) sets the length scale of the moiré pattern which has a periodicity of \( \frac{2\pi}{\delta K} \). The above Hamiltonian has the interesting property that the bandwidth of the low-energy bands depends on the parameter \( \alpha = \frac{\gamma_0}{\delta K} \). As \( \alpha \) increases from zero, the bandwidth decreases, approximately vanishes at \( \alpha \sim 1 \), and increases again with further increase in \( \alpha \). While a reduction in the bandwidth can be analytically understood by employing a perturbation theory in \( \alpha \), the quasiflat-band regime can be explored only numerically because perturbation theory breaks down when \( \alpha \sim 1 \).

To obtain an understanding of magic-angle TBG, it is imperative we ascertain which aspect(s) of the above Hamiltonian is(are) responsible for the phenomenon of band flattening. Are Dirac dispersion and band touching necessary? Is it essential for \( h_{1,2} \) and \( h_{\perp} \) to have a
Fig. 1. (a) Pictorial representation of the auxiliary Hamiltonian defined by Eqs. (3) and (4) (continuum model) or Eq. (6) with \( U = 0 \). Here \( t = 1 \) and \( \gamma_0 = \gamma_0[1 + g \cos(2\pi j/J)]e^{i(2\pi x/j)} \) with \( g = 0.1 \) and \( J = 6 \). With increase in \( \gamma_0 \), the lowest band first becomes quasiflat and then becomes dispersive. (c) Dependence of the bandwidth of the lowest band on \( \gamma_0 \). (d) Schematic representation of the origin of the low-energy quasiflat band—see text for description.

matrix structure (arising from the sublattice degrees of freedom)? Is the phenomenon constrained to only two dimensions? Motivated by these questions, we construct an auxiliary Hamiltonian by replacing Eqs. (1) and (2) with

\[
\begin{align*}
    h_{1,2} &= -\frac{\partial^2}{2m}, \\
    h_\perp &= \gamma(x)e^{i\phi(x)}. 
\end{align*}
\]

The auxiliary Hamiltonian is a priori unrelated to the original TBG Hamiltonian but the inspiration is obvious: We have replaced the individual graphene layers with one dimensional free electrons while keeping the coupling term complex similar to the TBG Hamiltonian. We impose the condition \( \gamma(x) = \gamma(x + X) \) and \( \phi(x) = \phi(x + X) \) so that \( h_\perp \) is periodic as in TBG. Thus, the auxiliary Hamiltonian is the long-wavelength limit of a two-leg ladder model threaded by a magnetic flux where the legs are coupled by a spatially varying periodic term, as represented in Fig. (a) (the corresponding lattice model is given by Eq. (6) with \( U = 0 \)). For simplicity, we assume a constant flux per plaquette and small spatial modulation of \( \gamma(x) \): \( \phi(x) = 2\pi x/X \equiv \phi_0 x \) and \( \gamma(x) = \gamma_0[1 + g \cos(2\pi x/X)] \), with \( g < 1 \).

We now show that the resulting low-energy band structure exhibits all the salient features of the bands in TBG. Fig. (b) shows that increasing \( \gamma_0 \), analogous to increasing \( \alpha \) in TBG, causes the bandwidth of the lowest-energy band to first decrease, go to a minimum resulting in a quasiflat band, and then increase again. This is summarized in Fig. (c). The mechanism leading to this behavior is traced schematically in Fig. (d): First, the complex interleg coupling causes the two degenerate bands to split along the momentum axis by an amount governed by the complex phase. Next, the constant part of the interleg coupling strength, \( \gamma_0 \), breaks the degeneracy at the touching point and separates out the low-energy band. Finally, the parameter \( g \), describing the spatially varying part of the coupling strength, opens up a gap \( \Delta_{BG} \) at the miniband edge due to Bragg scattering and separates out a quasiflat miniband of bandwidth \( \delta_{BW} \).

In momentum space, the low-energy bands are described by the truncated Hamiltonian,

\[
H_k = \begin{pmatrix}
    \varepsilon_{k,-1} & \gamma_0 & 0 & 0 \\
    \gamma_0 & \varepsilon_{k,0} & g\gamma_0/2 & 0 \\
    0 & g\gamma_0/2 & \varepsilon_{k,0} & \gamma_0 \\
    0 & 0 & \gamma_0 & \varepsilon_{k,+1}
\end{pmatrix},
\]

where \( \varepsilon_{k,n} = \frac{(k+n\phi_0)^2}{2m} \). Eq. (5) reproduces the band structure in Fig. (b) remarkably well, even in the quasiflat regime when \( \delta_{BW} \ll \Delta_{BG} \)—see supplemental material [10]. The band flattening results from a combined effect of the parameters \( \gamma_0 \) and \( g \) (for a fixed \( \phi_0 \)) which can be independently tuned in our model.

Since the flatness depends only on the flux and the spatially varying coupling term, one can replace the two legs of the ladder with any other object with required attributes (e.g., dimensionality, topology, internal degrees of freedom, etc.) which will be conferred on the resulting quasiflat band(s). This separation of effects can be exploited to design new quasiflat bands.

We now study the effect of interparticle interaction on the auxiliary Hamiltonian. While earlier works on related models studied the dispersive regime [17–19], here we focus on the quasiflat-band regime. To that end, we write
down the corresponding lattice version:

\[ H = -t \sum_{j,\sigma,\lambda} c_{j+1,\sigma,\lambda}^\dagger c_{j,\sigma,\lambda} + \sum_{j,\sigma} \gamma_j c_{j,\sigma,1}^\dagger c_{j,\sigma,1} + \text{h.c.} \]
\[ + U \sum_{j,\lambda} n_{j,\lambda} n_{j+1,\lambda}. \]

(6)

Here, \( c_{j,\sigma,\lambda} \) annihilates an electron on site \( j \), on the leg with index \( \lambda = 1, 2 \) and spin \( \sigma = \downarrow, \uparrow \). Hopping between adjacent sites in each leg is parametrized by \( t \) and between the two legs by \( \gamma_j = \gamma_0 \left( 1 + g \cos \frac{2\pi j}{J} \right) e^{i\frac{2\pi j}{J}}, \) where \( \gamma_0 \) and \( g \) are constants. In our calculation, we choose \( J \) to be 6 without any loss of generality, and set \( t = 1 \) to fix the energy scale. The first line reduces to Eqs. (4) and (5) in the long-wavelength limit. Interaction is added via an onsite Hubbard interaction of strength \( U \) in the second line, where \( n_{j,\sigma,\lambda} \) is the electron number operator. We are interested in the scenario when the quasiflat band is half-filled; therefore, we fix the electron density at \( n = \frac{1}{2} \).

The ground state properties are calculated using the finite-size Density Matrix Renormalization Group (DMRG) method \cite{20, 22} with open boundary conditions. Calculations are performed using the ITensor library \cite{23}. To minimize finite-size effects, we study systems of various sizes up to \( 2L = 2 \times 240 \) sites with cutoff error less than \( 10^{-9} \). The energy difference between two sweeps is less than \( 10^{-7} \) during final sweeps. Total charge- and \( S_z \)-conservation are implemented for better convergence \cite{10}.

In order to stay in the quasiflat-band regime we fix \( \gamma_0 = 0.49 \) and \( g = 0.1 \) so that \( \delta_{BW} \approx 7.5 \times 10^{-3} \) and \( \Delta_{BG} \approx 4.89 \times 10^{-2} \). For the Hubbard term, we impose the condition \( \delta_{BW} \lesssim \langle U \rangle < \Delta_{BG} \), where \( \langle U \rangle = U \sum_{j,\lambda} \langle n_{j,\lambda} n_{j,\lambda} \rangle \) is measured in the non-interacting limit. We choose \( U = 0.4 \) which gives \( \langle U \rangle / \Delta_{BG} \approx 0.18 \) and \( \langle U \rangle / \delta_{BW} \approx 1.17 \). As shown in Fig. 2(a), as a result of interaction a commensurate charge density wave emerges with the period of \( J \). To identify whether the phase is gapped or not, we calculate the charge gap defined as \( \Delta_c = \lim_{L \to \infty} \left[ E_0 (N_e = N + 2) - E_0 (N_e = N - 2) - 2E_0 (N_e = N) \right] \), where \( E_0 (N_e) \) refers to the ground state energy of a given electron number \( N_e \). We find \( \Delta_c = 0.0214 \), obtained after accounting for the finite-size scaling (see supplemental material \cite{14}). The charge gap increases monotonically as \( U \) increases, and saturates at \( \Delta_c = 0.0474 \) when \( U > 1 \), as shown in Fig. 2(b). Also, it is seen that \( \Delta_c \) goes to zero at \( U \approx 0.1 \), signaling a metal-insulator transition. The spin gap is defined similarly as \( \Delta_s = E_0 (S^{\text{tot}}_z = 1) - E_0 (S^{\text{tot}}_z = 0) \) because of the spin U(1) symmetry. We find that \( \Delta_s = 0 \) (less than \( 10^{-6} \)). The nonzero charge gap and a zero spin gap at finite \( U \) is consistent with the expectation that the system at half-filling is a Mott state.

We next investigate the spin-spin correlation in this Mott state. The spin-spin correlation within each leg is defined as \( \langle \vec{S}_{i,\lambda} \cdot \vec{S}_{j,\lambda} \rangle \), where \( \vec{S}_{i,\lambda} \) is the total spin of the electrons on site \( i \) of the \( \lambda \)-th leg. As shown in Fig. 2(c), the spin-spin correlation oscillates with the same period as the electron density. However, it is not a conventional spin density wave: the spin-spin correlation values are all positive between any two sites, indicating a ferromagnetic ordering. That is, ordering both within a supercell as well as between two supercells is ferromagnetic. A similar behavior is observed for the spin-spin correlation between the two legs, although it is found to be weaker than the intra-leg correlation. This is shown in Fig. 2(d). Note that the ordering is quasi-long range since a true long-range order is forbidden in 1D by the Mermin-Wagner theorem \cite{24}. In all, this suggests that in the quasiflat regime, the system is an unusual ferromagnetic Mott insulator.

It is natural to ask what happens to this phase when the band is no longer quasiflat. To address this, we keep the interaction strength unchanged but change the bandwidth by changing \( \gamma_0 \) while keeping \( g \) and \( \phi_0 \) fixed to the values used before. Thus, \( \gamma_0 \) is a proxy for the bandwidth which can be read off from Fig. 1(c). As shown in Fig. 3(a), as \( \gamma_0 \) is decreased (bandwidth is increased), the intra-leg spin-spin correlation changes...
FIG. 3. Effect of increasing the bandwidth by decreasing $\gamma_0$ on the ground state properties shown in Fig. 2 (a) The intraleg spin-spin correlation changes from ferromagnetic to antiferromagnetic as $\gamma_0$ decreases (bandwidth increases). The inset shows the correlations in the limit when the two legs are uncoupled. (b) The spin structure factor for various $\gamma_0$. The peaks at $k = 0$ are due to the non-zero average value of the correlations. The $k = 0$ peak is tallest for the flattest band (largest $\gamma_0$). (c) Same as in (a) but for interleg spin-spin correlation. (d) The charge gap at various values of $\gamma_0$ (bandwidths) after the finite-size scaling. All parameters used, except $\gamma_0$, are the same as those used in Fig. 2.

from ferromagnetic to antiferromagnetic. In the inset, we show the spin-spin correlation in the limit when the two legs are completely uncoupled. Once the transition has occurred, the spin-spin correlation quickly assumes the antiferromagnetic form expected for a single chain. Thus, the emergence of the ferromagnetic phase is contingent on a small bandwidth. A better representation of the ferromagnetic–antiferromagnetic transition can be achieved by computing the structure factor $S(k) = \frac{1}{N} \sum_{i,j} \langle \mathbf{S}_{i,\lambda} \cdot \mathbf{S}_{j,\lambda} \rangle e^{i(k(x_i - x_j))}$. We plot in Fig. 3(b) $S(k)$ vs. $k$ for different values of $\gamma_0$. Ferromagnetic ordering is indicated by sharp peaks at $k = 0$ and $k = 2\pi/6 = 2\pi/J$, which give way to antiferromagnetism at smaller $\gamma_0$ (larger bandwidth) as signaled by a sharp peak at $k = 2\pi/12 = \pi/J$. Around $\gamma_0 \approx 0.43$, where the transition happens, we find both peaks to be sharp. The ferromagnetic-to-antiferromagnetic transition is also observed in spin-spin correlation between the two legs as shown in Fig. 3(c). Finally, in the charge sector, we find charge density waves with the same periodicity as in the quasiflat band regime. The charge gap decreases with decrease in $\gamma_0$ (increase in bandwidth), as shown in Fig. 3(d), except near $\gamma_0 = 0.43$ where it shows certain features. This is the same value at which the ferromagnetic-antiferromagnetic transition appears in the spin sector.

We have confirmed that the above observations do not change qualitatively on introducing an additional nearest neighbor interaction term of the form $V \sum_{i,j,\sigma,\sigma',\lambda} n_i \sigma n_j \sigma' n_{i+1} \sigma' \lambda$ in Eq. (1)—see supplemental material (16).

We now discuss the relevance of these findings in the context of TBG. Experiments have found that near the magic angle, at half-filling of either the conduction or the valence bands, TBG becomes a correlated insulator [4, 6]. Recent theories have proposed that the ground state should be ferromagnetic [25, 26]. This has been attributed to the unusual shape of the Wannier functions for the quasiflat bands and an interplay between the spin and valley degrees of freedom. It is interesting that a ferromagnetic insulating state is also favored in our auxiliary model. Note that while our auxiliary model mimics TBG at the single particle level, the similarity is only in the energetics of the bandwidth, with a completely different microscopic structure—there is no Dirac physics, no valley degree of freedom, and our model is 1D as opposed to 2D—indicating that, perhaps, the underlying physics is quite general. Experimentally, no signature of ferromagnetism has yet been observed at half-filling in TBG. This could be due to the stringent requirement of the narrow bandwidth, so that TBG even slightly away from the magic angle has tendencies toward $k \neq 0$ spin density waves. On the other hand, ferromagnetism has been found recently at three-quarters filling of the conduction band through the observation of anomalous Hall effect [7]. It would be interesting, therefore, to extend our model to three quarters and other rational fillings of the band, and also include a valley degree of freedom; the latter can be achieved simply by considering two copies of the two-leg ladder, threaded by flux in opposite directions.

Beyond TBG, our model is relevant in the larger context of 1D correlations and magnetism. The emergence of ferromagnetism in the quasiflat regime of our model [Fig. 2(a)] seems to contradict the theorem by Lieb and Mattis which states that the ground state in 1D has the lowest possible spin $\frac{1}{2}$ [27, 28]. However, the proof assumes all hoppings and interactions to be real, which is not true in our model. Also, our model should be compared with Tasaki’s model [29, 30] which is known to give rise to flatband ferromagnetism: Tasaki’s model achieves flat bands by having more than one type of atom in the unit cell and beyond-nearest-neighbor-hopping whereas we achieve flat bands with strictly nearest neighbor hopping by including a flux. Similarly, the metal-insulator (Mott) transition at nonzero $U$ [Fig. 2(b)] is at odds with the general result that in 1D such a transition is
not expected \cite{31}. The latter is, however, valid only for cases with SU(2) symmetry—it is known to break down in SU(N) generalizations of the 1D Hubbard model \cite{32}. Considering the two legs in our model as pseudospins, it is then not surprising that we find a metal-insulator transition at nonzero $U$. Nevertheless, the role of the complex hopping term in this respect cannot be overruled. We are not aware of a theory that can adequately describe the model discussed here. A theory explaining the numerical findings will not only provide a basic understanding of many of the observed features in magic-angle TBG, it will also provide a novel direction in the study of 1D correlations and magnetism. These ideas can be experimentally tested independently using cold atoms where Fermionic flux ladders can be simulated \cite{33}.

In summary, we have shown that a two-leg ladder threaded by a flux with the legs coupled by a spatially varying periodic term produces a low energy quasiflat band with characteristics similar to that in magic angle TBG. In the presence of interactions, the ground state is a ferromagnetic Mott insulator, which gives way to an antiferromagnetic Mott insulator as the band becomes more dispersive. In addition to providing clues to the physics of magic angle TBG, our model is relevant in the larger context of 1D correlations and magnetism.

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SUPPLEMENTAL MATERIAL

The auxiliary Hamiltonian truncated in momentum space

The noninteracting auxiliary Hamiltonian is defined as (ignoring spin)

\[ H = -t \sum_j (c_{j+1,1}^\dagger c_{j,1} + \text{h.c.}) - t \sum_j (c_{j+1,2}^\dagger c_{j,2} + \text{h.c.}) + \sum_j (\gamma_j c_{j,1}^\dagger c_{j,1} + \text{h.c.}), \]  

(7)

where \( \gamma_j = \gamma_0 (1 + g \cos \phi_j) e^{i \phi_j} \), with \( \phi_j = \frac{2 \pi j}{L} \). We make the following gauge transformations: \( c_{j,1} \rightarrow c_{j,1} \) and \( c_{j,2} \rightarrow e^{i \phi_j} c_{j,2} \), and then carry out a Fourier transform: \( c_{j,\alpha} = \frac{1}{\sqrt{N}} \sum_k e^{ik \phi_j} c_{k,\alpha} \). Eq. (7) then becomes

\[ H = -2t \sum_k \cos(k) c_{k,1}^\dagger c_{k,1} - 2t \sum_k \cos(k + \phi_0) c_{k,2}^\dagger c_{k,2} + \gamma_0 (1 + g \cos \phi_0) \sum_k (c_{k,2}^\dagger c_{k,1} + \text{h.c.}) \].

(8)

Since we are interested only in the low-energy spectrum for \( k \in [-\phi_0/2, \phi_0/2] \), we can truncate the Hamiltonian in momentum space and write \( H = \sum_k H_k \) with

\[ H_k = \begin{pmatrix} c_{k,-\phi_0,1}^\dagger & c_{k,\phi_0,2}^\dagger & c_{k,1}^\dagger & c_{k,2}^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon_{k,-1} & \gamma_0 & 0 & 0 \\ \gamma_0 & \varepsilon_{k,0} & \gamma_0/2 & 0 \\ 0 & \gamma_0/2 & \varepsilon_{k,0} & \gamma_0 \\ 0 & 0 & \gamma_0 & \varepsilon_{k,+1} \end{pmatrix} \begin{pmatrix} c_{k,-\phi_0,1} \\ c_{k,\phi_0,2} \\ c_{k,1} \\ c_{k,2} \end{pmatrix}, \]

(9)

where \( \varepsilon_{k,n} = -2t \cos(k + n\phi_0) \) which in the long-wavelength limit becomes \( \frac{(k+n\phi_0)^2}{2m} \) with \( m = \frac{1}{2t} \) (discarding the constant shift of energy equal to \(-2t\)). As seen in Fig. 4, Eq. (9) reproduces the band structure obtained from Eq. (7) remarkably well, even in the quasiflat-band regime.

The convergence of numerical results

The convergence of the Density Matrix Renormalization Group (DMRG) results can be checked by the truncation error and ground state energy with increased number of states kept. As shown in Fig. 5, the ground state energy \( E_0 \) remains almost unchanged as the number of states increases, indicating that the numerical results are converged. Meanwhile the local spin value \( \langle S_z^c \rangle \) remains zero with an error bar in the order of the truncation error for any finite \( U \).

The finite-size scaling of the charge gap

The charge gap is defined as \( \Delta_c(U) = E_0(N_c = N + 2) + E_0(N_c = N - 2) - 2E_0(N_c = N) \). The calculations of the charge gap depend only on the ground state energy; thus, they are very reliable. Fig. 6 shows the finite-size scaling of the charge gap. The charge gap remains finite after the scaling for \( U > 0.2 \), which indicates a gapped phase.

![Fig. 4](image-url)  

**FIG. 4.** Comparison of the low-energy bands of the auxiliary Hamiltonian derived from exact tight-binding calculation (blue) and from the truncated Hamiltonian [Eq. (9)] (red). Here, \( t = 1 \), \( \phi_0 = 2\pi/6 \), and \( g = 0.1 \).
The spin correlations under the next-nearest-neighbor interactions

Besides the onsite Hubbard interactions, we have tested other interactions such as the next-nearest-neighbor Coulomb interactions, which is defined as $V \sum_{j, \sigma, \sigma'} n_{j, \sigma} n_{j+1, \sigma'}$. As shown in Fig. 7, the spin correlations become ferromagnetic for finite $V$, which is similar to the one with only onsite Coulomb interactions, suggesting that the ferromagnetic Mott state is robust against various types of Coulomb interactions.
FIG. 6. The finite-size scaling of the charge gap for various $U$ in the quasi-flat band regime. We have used a least-square fit to the third order of polynomials in $1/L$. Similar fittings are used in the extrapolation of the charge gap for various $\gamma_0$.

FIG. 7. The intra-chain spin correlations with next-nearest-neighbor Coulomb interactions, obtained for the system of length $L = 144$. We choose $x = \frac{L}{4}$ in order to minimize the effect of the open boundary. Only one leg is shown, the other is the same.