

Ground state of graphite ribbons with zigzag edges

Yu-Li Lee*

Division of Nanoscience, National Center for High-performance Computing, Hsinchu, Taiwan, Republic of China

Yu-Wen Lee†

Physics Department, Tunghai University, Taichung, Taiwan, Republic of China

(Received 20 June 2002; revised manuscript received 26 September 2002; published 4 December 2002)

We study the interaction effects on the ground state of nanographite ribbons with zigzag edges. Within the mean-field approximation, we find that there are two possible phases: the singlet superconducting (SS) phase and the excitonic insulator (EI) phase. The two phases are separated by a first-order transition point. After taking into account the low-lying fluctuations around the mean-field solutions, the SS phase becomes a spin liquid phase with one gapless charge mode. On the other hand, all excitations in the EI phase, especially the spin excitations, are gapped.

DOI: 10.1103/PhysRevB.66.245402

PACS number(s): 73.22.Gk, 73.22.-f, 73.22.Lp, 71.35.-y

I. INTRODUCTION

After the discovery of low-dimensional materials such as fullerenes and carbon nanotubes, the research on sp^2 network systems has been attracting much attention. The nanographite ribbon is one of the most simple and fundamental fragments of the sp^2 network, and represents an interesting class of mesoscopic systems. In this system the boundary regions play an important role, so that the edge effects may influence strongly the π -electron states near the Fermi surface.

There are two basic shapes of regular graphite edges—zigzag and armchair edges (see Fig. 1). The study of electronic states of hydrogen-terminated graphite ribbons reveals that ribbons with zigzag edges possess partly flat bands at the Fermi level, which correspond to the electronic states localized in the near vicinity of the edges.¹⁻³ In particular the highest valence band and the lowest conduction band are always degenerate at $ka_0 = \pi$, with the lattice spacing $a_0 \approx 2.46 \text{ \AA}$. (Hereafter we will set $a_0 = 1$.) The localized edge states are of special interest because of their relatively large contribution to the density of states at the Fermi surface, which results in the Curie-like temperature dependence of the Pauli susceptibility² and zero-conductance resonances in the nanographite ribbon junctions.⁴ It was reported that zigzag ribbons do not undergo bond alternations along the ribbon axis for a reasonable strength of electron-phonon interactions, because of the nonbonding character of the edge states.⁵ In other words, the partly flat bands are stable against the Peierls instability. In addition, the flat edge states exist not only in the single-layered zigzag ribbons but also in stacked layers of zigzag ribbons in a manner of the *AB* stacking,³ in which half of the carbon atoms of one ribbon are located directly above the center of each hexagon on the neighboring ribbons.

In this paper, we are interested in the low-energy physics of graphite ribbons with zigzag edges. In this case, it suffices to consider edge states only. A simple power counting indicates that all four-fermion interactions are relevant operators around the free-fermion fixed point (see Sec. III). Therefore, we expect that the electron-electron interactions will change

the free-fermion picture drastically. Based on a renormalization group analysis, we propose a model Hamiltonian with an $O(4)$ symmetry to describe the low energy physics of this system. A mean-field treatment of this Hamiltonian results in two possible zero temperature phases—singlet superconducting (SS) and excitonic insulator (EI) phases separated by a first-order transition point. For the EI phase,⁶ the singlet and triplet excitonic order parameters can coexist due to the underlying $O(4)$ symmetry.⁷ As a result, there is a degeneracy for the onset of the charge density wave and spin density wave ordering within the mean-field approximation. However, in one dimension, the low-lying fluctuations around the mean-field solutions are so strong that the long range orders obtained by the mean-field theory are destroyed and the true ground states exhibit algebraic (SS) or short-ranged (EI) orders. Consequently, the SS phase becomes a spin liquid with one gapless charge mode, whereas the EI phase turns into an insulating phase in which all excitations are gapped and the broken $O(4)$ symmetry is restored.

The rest of the paper is organized as follows: In Sec. II, we give a description of the system and discuss the action describing the dynamics of the flat edge states. We present

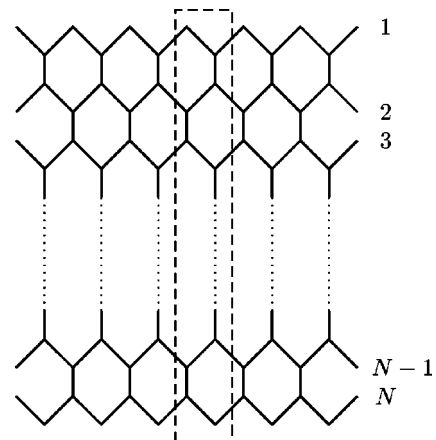


FIG. 1. The structure of graphite ribbons with zigzag edges. The carbon atoms are located at the corners of each hexagons. The rectangle with the dashed line is the unit cell.

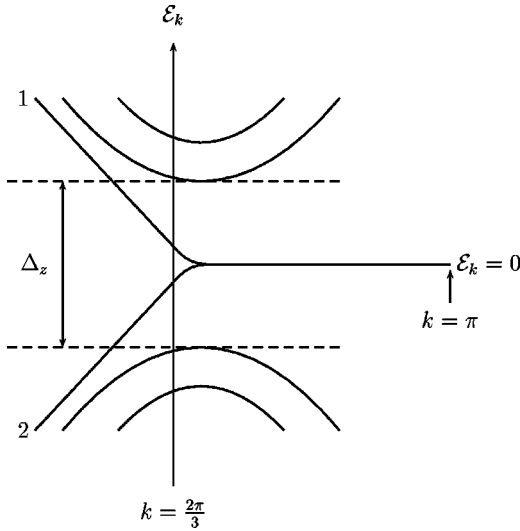


FIG. 2. The schematic figure of the energy band dispersion near $E=0$. Δ_z is given by Eq. (2). The band indices 1 and 2 indicate the two lowest bands.

the renormalization group (RG) analysis of the action in Sec. III, and propose an effective Hamiltonian which describes the low energy physics. The mean-field theory and the derivation of low-energy effective actions are given in Secs. IV and V, respectively. Section VI is devoted to discussions and conclusions.

II. MODEL SYSTEM

The structure of the graphite ribbon with zigzag edges and the schematic figure of its energy band dispersion near $E=0$ are shown in Figs. 1 and 2, respectively. The almost flat bands appear within the region $2\pi/3 \leq |k| \leq \pi$. For an H-terminated single-layered zigzag ribbon, the dispersion relations of the two lowest bands close to $k=\pi$ obtained from the tight-binding model has the approximate form^{1,2}

$$\mathcal{E}_{1(2)k} = \pm 2tND_k^{N-1} \left(1 - \frac{D_k}{2} \right), \quad (1)$$

where $D_k = 2 \cos(k/2)$, t is the hopping matrix element, and N is the number of zigzag lines (see Fig. 1). Equation (1) indicates that the two lowest bands are degenerate at the Fermi point $k=k_0=\pi$. Around that point, $\mathcal{E}_{1(2)k} \approx \pm 2Nt|k-k_0|^{N-1}$. The energy gap to the next band Δ_z , as shown in Fig. 2, is given by^{1,2}

$$\Delta_z = 4t \cos \left[\frac{(N-1)\pi}{2N+1} \right]. \quad (2)$$

Since the energy scale we are considering is much lower than Δ_z , only these two lowest bands are involved and the electron operator can be expanded around the Fermi point k_0 ,

$$\Psi_\alpha(\vec{x}) \approx e^{ik_0x} [\psi_{1\alpha}(x)u_1(y) + \epsilon_{\alpha\beta}\psi_{2\beta}^\dagger(x)u_2(y)], \quad (3)$$

such that $\psi_{a\alpha}|0\rangle=0$, where $a=1,2$ is the band index, and $\alpha=\pm 1$ corresponds to spin up and down, respectively. (We assume that the x axis is parallel to the ribbon axis.) The ψ

fermions describe the low-energy degrees of freedom. $u_{1,2}(y)$ are real functions which satisfy the orthonormal condition: $\int dy u_a(y)u_b(y) = \delta_{ab}$. Under the operation of reflection about the line along the ribbon axis at the middle of the ribbon, denoted by a unitary operator \mathcal{R} , we have $\mathcal{R}u_1 = u_2$. (Note that this results in $u_1^2 = u_2^2$.)

Up to the four-fermion interactions, the most general form of the action describing the dynamics of ψ fermions in the imaginary-time formulation is given by

$$I = I_0 + \int d\tau dx L_1,$$

where

$$I_0 = \int \frac{d\omega}{2\pi} \int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} \tilde{\psi}_{a\alpha}^\dagger(-i\omega + v|k|^m) \tilde{\psi}_{a\alpha}, \quad (4)$$

$$L_1 = \frac{g_1}{2} (\rho_1^2 + \rho_2^2) + g_2 \rho_1 \rho_2 + 4g_3 \mathbf{J}_1 \cdot \mathbf{J}_2 + g_4 (N_1 N_2 + \text{H.c.}). \quad (5)$$

Here $\tilde{\psi}_{a\alpha}(\vec{k}) \equiv \int dx e^{-ik \cdot \vec{x}} \psi_{a\alpha}(\vec{x})$, $m > 1$ ($m = N - 1$ for the single-layered graphite ribbons), $v = 2Nt$, Λ is an UV cutoff for the momentum, and

$$\begin{aligned} \rho_a &= \psi_{a\alpha}^\dagger \psi_{a\alpha}, \\ \mathbf{J}_a &= \frac{1}{2} \psi_{a\alpha}^\dagger (\boldsymbol{\sigma})_{\alpha\beta} \psi_{a\beta}, \\ N_a &= \frac{i}{2} \epsilon_{\alpha\beta} \psi_{a\alpha} \psi_{a\beta}. \end{aligned} \quad (6)$$

In Eq. (4), we have replaced $k - k_0$ by k . ρ_a , \mathbf{J}_a , and N_a , defined above, are, respectively, the charge density, the spin density, and the singlet Cooper pair in the band a . g_1 is the intraband interaction, and the interband interactions are described by the density-density interaction g_2 , the exchange interaction g_3 , and the singlet Cooper-pair tunneling g_4 . (Note that the triplet Cooper-pair tunneling term vanishes in the present case because of the Fermi statistics.) We have to emphasize that, regardless of the graphite ribbons being H terminated, not H terminated, single layered, or stack layered, Eqs. (4) and (5) describe the dynamics of the flat edges states as long as they exist. The short distance structure only affects the values of the parameters g_i ($i=1, \dots, 4$), v , and m , which will ultimately determine in which phase the system is located.

To obtain the values of the couplings g_i ($i=1, \dots, 4$), we consider the short-ranged electron-electron interactions described by the interacting Hamiltonian

$$\begin{aligned} H_{int} &= \frac{1}{2} \int d^2x_1 d^2x_2 : \Psi_\alpha^\dagger(\vec{x}_1) \Psi_\beta^\dagger(\vec{x}_2) \\ &\quad \times V(\vec{x}_1 - \vec{x}_2) \Psi_\beta(\vec{x}_2) \Psi_\alpha(\vec{x}_1) :. \end{aligned} \quad (7)$$

By inserting Eq. (3) into Eq. (7), we obtain

$$g_1 = U_1(0), \quad g_2 = -U_1(0) + \frac{U_2(0)}{2},$$

$$-2g_3 = U_2(0) = g_4, \quad (8)$$

where $U_i(q) = \int dx e^{-iqx} V_i(x)$ ($i=1,2$), and

$$V_1(x_1 - x_2) = \int dy_1 dy_2 u_1^2(y_1) V(\vec{x}_1 - \vec{x}_2) u_1^2(y_2),$$

$$V_2(x_1 - x_2) = \int dy_1 dy_2 u_1(y_1) u_2(y_1)$$

$$\times V(\vec{x}_1 - \vec{x}_2) u_1(y_2) u_2(y_2).$$

Especially for a Hubbard-like interaction $V(\vec{x}_1 - \vec{x}_2) = V_0 \delta(\vec{x}_1 - \vec{x}_2)$, we have $g_1 = U = -2g_2 = -2g_3 = g_4$ where $U = V_0 \int dy u_1^4(y)$. We see that $g_1, g_4 > 0$ and $g_2, g_3 < 0$ when the interactions between electrons are repulsive.

The symmetries of the action I are the charge $U(1)$ [denoted by $U_c(1)$] where the ψ fermions transform as $\psi_{1\alpha} \rightarrow e^{i\theta} \psi_{1\alpha}$ and $\psi_{2\alpha} \rightarrow e^{-i\theta} \psi_{2\alpha}$; the spin $SU(2)$; and Z_2 (particle hole), where the ψ fermions transform as $\psi_{1\alpha} \leftrightarrow \psi_{2\alpha}$. In this paper, we restrict ourselves to the undoped case. The chemical potential term breaks the Z_2 symmetry and thus will not be generated by renormalization.

III. RENORMALIZATION GROUP ANALYSIS

We first show that L_1 is a relevant perturbation to the free-fermion action I_0 . By integrating out the fast modes with $\Lambda/s < |k| < \Lambda$, we find that I_0 is a fixed point of the RG transformation

$$k \rightarrow k/s, \quad \omega \rightarrow \omega s^{-m}, \quad \tilde{\psi}_{a\alpha} \rightarrow \xi \tilde{\psi}_{a\alpha}, \quad (9)$$

with $\xi = s^{m-1/2}$. Under the RG transformation [Eq. (9)], the couplings in L_1 transform as $g'_i = s^{m-1} g_i$ ($i=1, \dots, 4$). We see that in one dimension all couplings are relevant and have the same scaling dimension around the free-fermion fixed point I_0 . To tell which terms dominate the low energy physics, a controllable approximation to organize the quantum fluctuations is necessary. Here we adopt the ϵ expansion.⁸ That is, we extend the spatial dimension from 1 to d and then use $\epsilon = d_u - d$ as the expansion parameter to compute the RG functions, where $d_u = m$ is the upper-critical dimension. For small N (and thus small m), the ϵ expansion may be reliable. For larger N , it is hoped that there is no qualitative difference in physical properties from small N to large N as long as N is finite.

Next we would like to examine the quantum fluctuations up to the one-loop order. Defining the dimensionless couplings $\lambda_i = \Lambda^{-\epsilon} c g_i / v$ ($i=1, \dots, 4$), where $c = S_{N-1} / [2(2\pi)^{N-1}]$ and S_d is the area of a d -dimensional sphere, and calculating the one-loop corrections to the coupling constants g'_i ($i=1, \dots, 4$), we obtain the one-loop RG equations within the ϵ expansion:

$$\frac{d\lambda_1}{dl} = \epsilon \lambda_1 - \lambda_1^2 - \lambda_4^2,$$

$$\frac{d\lambda_2}{dl} = \epsilon \lambda_2 - \lambda_2^2 - 3\lambda_3^2 - \lambda_4^2,$$

$$\frac{d\lambda_3}{dl} = \epsilon \lambda_3 - 2\lambda_3(\lambda_2 - \lambda_3), \quad (10)$$

$$\frac{d\lambda_4}{dl} = \epsilon \lambda_4 - 2\lambda_4(\lambda_1 + 2\lambda_2).$$

Equation (10) is solved numerically up to a scale l^* , at which point the largest coupling $\lambda_{max} = \max\{\lambda_i(l^*)\}$ satisfies $\tilde{U} \ll \lambda_{max} \ll 1$, where $\tilde{U} \equiv \Lambda^{-\epsilon} c U / v$. This allows us to ignore the higher-order terms [$O(\lambda_i^3)$] in the RG equations. As $\tilde{U} \rightarrow 0$, $l^* \rightarrow \infty$, and we need only analyze the asymptotic large l behaviors of Eq. (10). We find that for $\epsilon > 0$, λ_2 and λ_4 become divergent first while the value of λ_1 approaches zero and that of λ_3 remains small when $\lambda_{2,4} = O(1)$.

Based on this analysis, we propose that the low-energy physics of the graphite ribbons with zigzag edges is described by the model Hamiltonian

$$H = \int \frac{dk}{2\pi} \epsilon_k \tilde{\psi}_{a\alpha}^\dagger(k) \tilde{\psi}_{a\alpha}(k) + \int dx [g(N_1 N_2 + \text{H.c.})$$

$$- \tilde{g} \rho_1 \rho_2], \quad (11)$$

where $g, \tilde{g} > 0$ and $\epsilon_k = v|k|^m$. The symmetry of H is $U_c(1) \times SU(2) \times SU(2) \times Z_2$ where the $SU(2) \times SU(2)$ symmetry corresponds to the independent spin rotations in each band. The enlarged symmetry [$SU(2) \rightarrow SU(2) \times SU(2)$] arises from the suppression of the g_3 term under the RG transformation. The values of g and \tilde{g} depend on v and the initial values of g_i 's ($i=1, \dots, 4$). Sec. IV, we shall treat the coupling constants g and \tilde{g} as free parameters and study the possible phases of Hamiltonian (11).

IV. MEAN-FIELD THEORY

The g term in Hamiltonian (11) describes the process of singlet Cooper-pair tunneling between two bands and favors the singlet superconductor when it becomes divergent, whereas a strong \tilde{g} term enhances the fluctuations of electron-hole pairs or excitonic ordering between band 1 and band 2.⁹ The latter can be represented by the singlet or triplet excitonic order parameters according to the angular momentum it carries. Motivated by this observation, we define the following order parameters:

$$\hat{O}_{sa}(x) = g \psi_{a\uparrow}(x) \psi_{a\downarrow}(x),$$

$$\Phi_s(x) = i \frac{\tilde{g}}{2} \epsilon_{\alpha\beta} \psi_{1\alpha}(x) \psi_{2\beta}(x), \quad (12)$$

$$\Phi_t(x) = \frac{\tilde{g}}{2} \epsilon_{\alpha\lambda} \psi_{2\lambda}(x) (\boldsymbol{\sigma})_{\alpha\beta} \psi_{1\beta}(x).$$

With the help of the Hubbard-Stratonovich transformation, the corresponding action of the Hamiltonian (11) in the imaginary-time formulation can be written as

$$S = \int \frac{d\omega}{2\pi} \frac{dk}{2\pi} \tilde{\psi}_{a\alpha}^\dagger (-i\omega + \epsilon_k) \tilde{\psi}_{a\alpha} + \int d\tau dx (\mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3), \quad (13)$$

where

$$\mathcal{L}_1 = \frac{1}{g} \hat{O}_{s1} \hat{O}_{s2} - \hat{O}_{s1} \psi_{2\uparrow} \psi_{2\downarrow} - \hat{O}_{s2} \psi_{1\uparrow} \psi_{1\downarrow} + \text{H.c.},$$

$$\mathcal{L}_2 = \frac{2}{\tilde{g}} |\hat{\Phi}_s|^2 - (i\hat{\Phi}_s^\dagger \epsilon_{\alpha\beta} \psi_{1\alpha} \psi_{2\beta} + \text{H.c.}),$$

$$\mathcal{L}_3 = \frac{2}{\tilde{g}} |\hat{\Phi}_t|^2 - (\hat{\Phi}_t^\dagger \cdot \epsilon_{\alpha\lambda} \psi_{2\lambda} (\boldsymbol{\sigma})_{\alpha\beta} \psi_{1\beta} + \text{H.c.}).$$

The mean-field treatment of the action S [Eq. (13)] is to assume the presence of bosonic mean fields, neglect the fluctuations of order parameters, and finally, integrate out the fermionic degrees of freedom to derive the effective potential. Now we consider the mean-field ansatz $O_{sa} = \langle \hat{O}_{sa} \rangle$, $\Phi_s = \langle \hat{\Phi}_s \rangle$, and $\Phi_t = \langle \hat{\Phi}_t \rangle$. The effective potential is given by

$$V = \frac{1}{g} (O_{s1} O_{s2} + \text{C.c.}) + \frac{2}{\tilde{g}} (|\Phi_s|^2 + |\Phi_t|^2) - \int \frac{d\omega}{2\pi} \frac{dk}{2\pi} \ln \left[\frac{F(\omega, k)}{F_0(\omega, k)} \right], \quad (14)$$

where $F_0(\omega, k) = (\omega^2 + \epsilon_k^2)^2$, and

$$F(\omega, k) = (\omega^2 + \epsilon_k^2)^2 + |O_{s1}^* O_{s2}^* + \Delta^T \Delta|^2 + (\omega^2 + \epsilon_k^2) (|O_{s1}|^2 + |O_{s2}|^2 + 2\Delta^\dagger \Delta).$$

Here $\Delta = (\Phi_s, \Phi_t)^T$ is the excitonic order parameter. In Eq. (14), we have set $V=0$ for free fermions.

The ground state is determined by the minimum of the effective potential V and the solutions of the mean-field equations are given by

$$O_{s1} = O_{s2}^* = \Delta_s e^{i\phi_0}, \quad \Delta = 0, \quad (15)$$

where $\Delta_s = C_m v^{-1/(m-1)} g^{m/(m-1)}$ with $C_m = a_m^{m/(m-1)}$ and $a_m = B[(1/2m, (1/2) - (1/2m)] / (4m\pi)$, and

$$\Delta = \Delta_0 e^{i\theta_0}, \quad O_{s1} = 0 = O_{s2}, \quad (16)$$

where Δ_0 is a real vector with the fixed length: $\Delta_e = \sqrt{\Delta_0^T \Delta_0} = C_m v^{-1/(m-1)} \tilde{g}^{m/(m-1)}$. Here $B(x, y)$ is the beta function. Solutions (15) and (16) correspond to the SS and EI phases, respectively. Especially in the EI phase, $\Phi_s \neq 0$ can coexist with $\Phi_t \neq 0$. It is well known^{9,10} that the singlet (Φ_s) and triplet (Φ_t) excitonic orders are accompanied by the appearance of charge and spin density waves. In our case, the onset of both ordering is degenerate on account of the $O(4)$ or $SU(2) \times SU(2)$ symmetry of action (13). The weak inter-

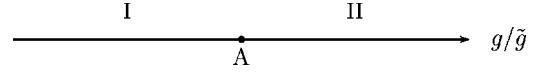


FIG. 3. The mean-field phase diagram. Region I is the EI phase and region II is the SS phase. The point A ($g = \tilde{g}$) is a first-order transition point.

actions which are neglected in Hamiltonian (11) will lift this degeneracy. A residual Coulomb interaction like the g_3 term favors the triplet excitonic order, while the electron-phonon interactions favor the singlet excitonic order.¹⁰ Note that naively the hidden symmetry of the EI phase is $U_f(1) \times O(4)$, where the $U_f(1)$ symmetry corresponds to the transformation: $\psi_{a\alpha} \rightarrow e^{i\tilde{\theta}} \psi_{a\alpha}$. However, it is not a symmetry of Hamiltonian (11) and we will see later that after taking into account the fluctuations the value of θ_0 cannot be arbitrary.

The point $g = \tilde{g}$ corresponds to the first-order phase transition because at that point the ground-state energies of the SS and EI phases are equal and the corresponding order parameters do not vanish. Thus the values of the order parameters change discontinuously from the SS to EI phases, or vice versa. This is consistent with the RG flow obtained from the ϵ -expansion. Since the RG equation (10) does not exhibit any IR stable fixed point, the phase transition cannot be the second-order one. To sum up, the zero-temperature phase diagram within the mean-field approximation is shown in Fig. 3.

V. LOW-ENERGY EFFECTIVE ACTION

To examine the stability of the mean-field solutions obtained above, we have to consider the fluctuations around the mean-field ground state. In the SS phase, \hat{O}_{s1} and \hat{O}_{s2} can be parametrized as $\hat{O}_{s1} = \Delta_s e^{i\phi_1}$ and $\hat{O}_{s2} = \Delta_s e^{-i\phi_2}$. On the other hand, the excitonic order parameter Δ becomes the ordinary bosonic field. Inserting these into action (13) and integrating out the fermionic fields and Δ , we obtain the low-energy effective theory in the SS phase,

$$\mathcal{L}_s = \frac{K_0}{2} \left[\frac{1}{v_s} (\partial_\tau \phi_+)^2 + v_s (\partial_x \phi_+)^2 \right] + \frac{\bar{K}_0}{2} \left[\frac{1}{v_s} (\partial_\tau \phi_-)^2 + \bar{v}_s (\partial_x \phi_-)^2 \right] + \mu_0 \cos \phi_-, \quad (17)$$

where $\phi_\pm = \phi_1 \pm \phi_2$, $K_0 = \bar{K}_0 = [(m-1)/2] \sqrt{a_m b_m}$, and $v_s = \bar{v}_s = m \sqrt{b_m / a_m} v^{1/m} \Delta_s^{1-(1/m)}$, and $b_m \propto (\Delta_z / \Delta_s)^{1-(1/m)} \gg 1$ is a nonuniversal constant. The ϕ_+ -field carries charge two and spin zero while the quantum numbers of ϕ_- are $Q=0$ and $S=0$. The cosine term in \mathcal{L}_s opens a gap in the ϕ_- sector because $\bar{K}_0 > (8\pi)^{-1}$. The charge $U(1)$ symmetry forbids the terms like $\cos(\beta\phi_+)$ or $\sin(\beta\phi_+)$. Therefore, the ϕ_+ sector remains gapless. After taking into account the fluctuations, the mean-field gap Δ_s becomes the spin gap and the SS phase is, in fact, a spin liquid phase with one gapless charge mode, which is similar to the $C1S0$ phase in the two-leg

Hubbard ladder.¹¹ In addition, the long range SS order turns into an algebraic one due to the gapless ϕ_+ -field, and the SS fluctuations are enhanced compared with the free fermions.

In the EI phase, the excitonic order parameter Δ can be written as: $\Delta = \Delta_e \Phi e^{i\theta}$ where Φ is a real vector satisfying $\Phi^T \Phi = 1$ and transforms with the fundamental representation of $O(4)$, whereas \hat{O}_{s1} and \hat{O}_{s2} are ordinary bosonic fields. The quantum numbers of the θ field are $Q=0$ and $S=0$ and the ones carried by the Φ sector consist of $(Q, S) = (0, 0)$ and $(0, 1)$. The low-energy effective theory in this case can be obtained by inserting the above parametrization into action (13) and integrating out the fermionic fields \hat{O}_{s1} and \hat{O}_{s2} , and then we have

$$S_{EI} = \int d\tau dx (\mathcal{L}_\theta + \mathcal{L}_\Phi),$$

where

$$\mathcal{L}_\theta = \frac{K}{2} \left[\frac{1}{v_e} (\partial_\tau \theta)^2 + v_e (\partial_x \theta)^2 \right] + \lambda \cos(2\theta), \quad (18)$$

$$\mathcal{L}_\Phi = \frac{\rho_o}{2} \left[\frac{1}{v_o} (\partial_\tau \Phi)^2 + v_o (\partial_x \Phi)^2 \right]. \quad (19)$$

Here $K = \rho_o = 2(m-1) \sqrt{a_m \bar{b}_m}$, $v_e = v_o = m \sqrt{\bar{b}_m / a_m} v^{1/m} \Delta_e^{1-(1/m)}$, and $\bar{b}_m \propto (\Delta_z / \Delta_e)^{1-(1/m)} \gg 1$ is a nonuniversal constant. In Eq. (18), we keep the leading cosine term only. Because $K > (2\pi)^{-1}$, the cosine term in \mathcal{L}_θ is a relevant operator and the θ sector acquires a gap. In addition, $\langle \theta \rangle$ is pinned at some value θ_0 which depends on the short distance physics. The dynamics of the Φ sector is described by the $O(4)$ nonlinear σ model. In general, there can be two sources to change the low-energy behavior of the nonlinear σ model. The first one is the existence of a term linear in $\partial_\tau \Phi$, which follows from the analysis of the equations of motion (EOM) and Ward identities.¹² As discussed in Ref. 12, the existence of this term relies on the nonvanishing expectation values of the corresponding conserved charges, i.e., $\langle \mathbf{J}_a \rangle \neq 0$ in the present case. But $\langle \mathbf{J}_a \rangle \neq 0$ implies the long range ferromagnetic order and it is forbidden in 1+1 dimensions by the Mermin-Wagner-Coleman theorem.¹³ The second one is the appearance of the θ -term, which results from the topological consideration and has no effects on the EOM. In our case, \mathcal{L}_Φ does not contain such a term because the homotopy group $\Pi_2[O(4)] = 0$. As a result, in the long wavelength limit, \mathcal{L}_Φ starts from the second derivatives of space and time as shown in Eq. (19). Therefore, the broken $O(4)$ symmetry is restored and the spectrum corresponding to the Φ sector is organized as the $O(4)$ multiplets. In addition, the corresponding excitations acquire an energy gap which is given by

$$\bar{\Delta}_s = c \Delta_e e^{-\pi \rho_0}, \quad (20)$$

where $c = O(1)$ is a non-universal constant. Because the charge excitations in this phase are associated with the fermion fields and $\bar{\Delta}_s \ll \Delta_e$, the mean-field gap Δ_e can be identified as the charge gap and the spin gap is determined by

$\bar{\Delta}_s$. Although the charge gap is not equivalent to the spin gap, there is no spin-charge separation in this phase. In conclusion, the long range excitonic order becomes a short-ranged one and all excitations are gapped.

A residual Coulomb interaction like the g_3 term in Eq. (5) leads to the breaking of the $O(4)$ symmetry and the mean-field theory favors $\Phi_i \neq 0$. Following a similar procedure, the Lagrangian which describes the corresponding low-lying fluctuations now consists of \mathcal{L}_θ as shown in Eq. (18) and the $O(3)$ nonlinear σ model. We have no arguments to exclude the possibility of the appearance of the θ term in the $O(3)$ nonlinear σ model as the case of the spin- $\frac{1}{2}$ Heisenberg chain. If a θ term exists, then the ground state will exhibit an algebraic long range triplet excitonic (spin density wave) order and the spin gap will vanish. On the other hand, if the θ term vanishes as the two-leg spin ladder, then the spin excitations still have a finite gap.

VI. CONCLUSIONS AND DISCUSSIONS

In the present paper, we study the low energy physics of the undoped nanographite ribbons with zigzag edges by neglecting the electron-phonon interactions. We show that the interactions between electrons substantially change the physics of the partly flat bands. According to the above analysis, there are two possible phases: a metallic phase with a spin gap (spin liquid) and enhanced SS correlations (region II in Fig. 3), and an insulating phase with a gapped spectrum (region I in Fig. 3). Our results that there are two possible phases are valid for both the cases of the single layer and AB stacking.¹⁴ In the latter case, the values of v , g , \tilde{g} , and the exponent m in Eq. (11) will be different from those in the single layer. Through these parameters v , g , \tilde{g} , and m , the material properties of the graphite ribbon determine in which phase this system is truly located.

To determine which one, the EI, the spin liquid, or the gapless edge states predicted by the band theory, is the ground state of the graphite ribbon with zigzag edges, we suggest two types of experiments: (i) the measurement of the single-particle density of states (DOS) by scanning tunneling microscopy, and (ii) the measurement of the uniform magnetic susceptibility. For the EI and spin liquid, the single-particle DOS vanishes when the energy is smaller than the spectral gap, which is distinguished from the gapless edge states predicted by the band theory, where the single-particle DOS still has a finite value at low energy. One of the distinctions between the spin liquid phase and the gapless edge states is the temperature dependence of the uniform magnetic susceptibility. At low temperature, it will exhibit an activated behavior in the spin liquid phase due to the spin gap, whereas the Curie-like behavior is expected for the gapless edge states.²

The enhanced SS fluctuations arise from the singlet Cooper-pair tunneling between two bands. It is also the origin of the spin liquid phase with strong SS correlations in many one-dimensional two-band models as emphasized in Ref. 15. In contrast, the excitonic fluctuations are suppressed after taking into account the quantum fluctuations. This re-

sults from a special feature of the broken non-Abelian symmetry in $1+1$ dimensions, where the corresponding nonlinear sigma model becomes IR unstable due to the lack of the topological term.

In the usual one-dimensional two-band electron system, the competing order of the singlet superconductor is the interchannel charge density wave (CDW),¹⁶ which also results from the same interaction as the \tilde{g} term in our Hamiltonian (11). The onset of the interchannel CDW requires the nearly equal electron density in the two bands. This is impossible in our case because, here, one band is empty and the other is completely filled.

Finally, we discuss the effects of electron or hole doping. For finite doping, the system may be described by the one-

band Luttinger liquid with a very small Fermi velocity. For lightly doping, the mean-field theory is supposed to be robust. Therefore, our results are not affected qualitatively. According to the analysis of Ref. 17 on the doped EI, there may be an inhomogeneous state between the EI and the Luttinger liquid upon increasing the doping concentration.

ACKNOWLEDGMENTS

Y.L.L. would like to thank M.F. Lin for discussions and Global fiberoptics, Inc. for financial support. The work of Y.-W.L. was supported by the National Science Council of Taiwan under grant NSC91-2112-M-029-012.

*Electronic address: c00lyl00@nchc.gov.tw

†Electronic address: ywlee@mail.thu.edu.tw

¹K. Nakada, M. Fujita, G. Dresselhaus, and M.S. Dresselhaus, Phys. Rev. B **54**, 17954 (1996).

²K. Wakabayashi, M. Fujita, H. Ajiki, and M. Sigrist, Phys. Rev. B **59**, 8271 (1999).

³Y. Miyamoto, K. Nakada, and M. Fujita, Phys. Rev. B **59**, 9858 (1999).

⁴K. Wakabayashi and M. Sigrist, Phys. Rev. Lett. **84**, 3390 (2000); K. Wakabayashi, Phys. Rev. B **64**, 125428 (2001).

⁵K. Wakabayashi, M. Sigrist, and M. Fujita, J. Phys. Soc. Jpn. **67**, 2089 (1998).

⁶For a review of the excitonic phase, see B.I. Halperin and T.M. Rice, Solid State Phys. **21**, 115 (1968).

⁷A discussion of the excitonic phase with the hierarchy of symmetry breaking $SU(4) \rightarrow SU(2) \times SU(2) \rightarrow SU(2) \times Z_2$ has appeared in the context of a strong interaction limit of the excitonic ordering. See L. Balents, Phys. Rev. B **62**, 2346 (2000).

⁸For the use of the ϵ expansion to perform a renormalization group analysis in the context of critical phenomena and quantum field theories, see, for example, J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Oxford University Press, Oxford,

1993).

⁹A.N. Kozlov and L.A. Maksimov, Zh. Éksp. Teor. Fiz. **48**, 1184 (1965) [Sov. Phys. JETP **21**, 790 (1965)].

¹⁰B.A. Volkov, Yu.V. Kopae, and A.I. Rusinov, Zh. Éksp. Teor. Fiz. **68**, 1899 (1975) [Sov. Phys. JETP **41**, 952 (1976)].

¹¹L. Balents and M.P.A. Fisher, Phys. Rev. B **53**, 12133 (1996).

¹²H. Leutwyler, Phys. Rev. D **49**, 3033 (1994).

¹³In $2+1$ or $3+1$ dimensions, $\langle J_a \rangle \neq 0$ is allowed. In that case, the term linear in $\partial_\tau \Phi$ can exist as the FM case and the dispersion relation of the Goldstone modes at long wavelength will behave as $\omega \sim |\vec{k}|^2$.

¹⁴A possible excitonic instability in a related system layered graphite, was suggested in D.V. Khveshchenko, Phys. Rev. Lett. **87**, 206401 (2001); **87**, 246802 (2001).

¹⁵V.J. Emery, S.A. Kivelson, and O. Zachar, Phys. Rev. B **59**, 15641 (1999).

¹⁶For a review about the various instabilities in the one-dimensional two-band electron systems, see O.A. Starykh, D.L. Maslov, W. Häusler, and L.I. Glazman, cond-mat/9911286 (unpublished).

¹⁷L. Balents and C.M. Varma, Phys. Rev. Lett. **84**, 1264 (2000); V. Barzykin and L.P. Gor'kov, *ibid.* **84**, 2207 (2000).