Spin-charge Separation in Nodal Antiferromagnetic Insulator

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In this paper, by using two dimensional (2D) Hubbard models with $\pi$-flux phase and that on a hexagonal lattice as examples, we explore spin-charge-separated solitons in nodal antiferromagnetic (AF) insulator - an AF order with massive Dirac fermionic excitations (see detail in the paper). We calculate fermion zero modes and induced quantum numbers on solitons (half skyrmions) in the continuum limit, which are similar to that in the quasi one-dimensional conductor polyacetylene (CH), and that in topological band insulator. In particular, we find some novel phenomena: thanks to an induced staggered spin moment, a mobile half skyrmion becomes a fermionic particle; when a hole or an electron is added, the half skyrmion turns into a bosonic particle with charge degree of freedom only. Our results imply that nontrivial induced quantum number on solitons may be a universal feature of spin-charge separation in different systems.

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The Fermi liquid based view of the electronic properties has been very successful as a basis for understanding the physics of conventional solids. The quasi-particles of Fermi liquid carry both spin and charge quantum numbers. However, in some cases, spin-charge separation occurs, providing a new framework for thinking about the given systems. It indicates that the systems have two independent elementary excitations, neutral spinon and spinless holon, respectively, as opposed to single quasi-particle excitation in conventional solids.

In condensed matter physics - one is an AF order on a honeycomb lattice, the other is $\pi$-flux phase together with a nonzero Neel order parameter. Based on these examples, our results confirm that induced quantum number on solitons is an important feature of the spin-charge separation in different systems.

Formulation— To develop a systematical formulation, we start with the extended Hubbard models,

$$H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} - \mu \sum_{i,\sigma} \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma} + h.c.$$  (1)

Here $\hat{c}^\dagger_{i,\sigma}$ and $\hat{c}_{j,\sigma}$ are electronic creation and annihilation operators. $U$ is the on-site Coulomb repulsion. $\sigma$ are the spin-indices for electrons, $\mu$ is the chemical potential. $\langle i, j \rangle$ denotes two sites on a nearest-neighbor link. $\hat{n}_{j\uparrow}$ and $\hat{n}_{j\downarrow}$ are the number operators of electrons with up-spin and down-spin. On a honeycomb lattice, the nearest neighbor hopping is a constant, $t_{ij} = t$; on a square lattice with $\pi$-flux phase, it can be chosen as $t_{i,i+x} = x$, $t_{i,i+y} = iy$.  The partition function of the extended Hubbard models is written as $Z = \int D\sigma D\psi e^{-\int_0^\beta d\tau L}$, where

$$L = \sum_{j, \sigma} \bar{c}_{j,\sigma} (\partial_\tau - \mu) c_{j,\sigma} + \sum_{\langle i,j \rangle, \sigma} t_{ij} \bar{c}_{i,\sigma} c_{j,\sigma}$$  (2)

$$-U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}.$$  (2)

$\bar{c}_{i,\sigma}$ and $c_{j,\sigma}$ are Grassmann variables describing the electronic fields.

Firstly let us derive long wave-length effective Lagrangian of the hopping term in the extended Hubbard models. Although $\pi$-flux phase does not break translational symmetry, we may still divide the square lattice into two sublattices, $A$ and $B$. After transforming the hopping term into momentum space, we obtain $E_f = 2\sqrt{\cos^2 k_x + \cos^2 k_y}$. So there exist two nodal fermi-points at $k_1 = (\frac{\pi}{2}, \frac{\pi}{2})$, $k_2 = (\frac{\pi}{2}, -\frac{\pi}{2})$ and the spectrum of fermions becomes linear in the vicinity of the two
nodal points. On a honeycomb lattice, after dividing the lattice into two sublattices, $A$ and $B$, the dispersion is obtained in Ref. [13, 16, 17]. There also exist two nodal points, $k_1 = \frac{2\pi}{\sqrt{3}} (1, \frac{1}{\sqrt{3}})$ and $k_2 = \frac{2\pi}{\sqrt{3}} (-1, -\frac{1}{\sqrt{3}})$ and the spectrum of fermions becomes linear near $k_{1,2}$. In the continuum limit, the Dirac-like effective Lagrangian describes the low energy fermionic modes for both cases

$$L_f = i\bar{\psi}_1\gamma_\mu \partial_\mu \psi_1 + i\bar{\psi}_2\gamma_\mu \partial_\mu \psi_2$$

where $\bar{\psi}_1 = \psi_{1,0}^\dagger = (\bar{\psi}_{1A}, \bar{\psi}_{1B}, \bar{\psi}_{1A}, \bar{\psi}_{1B})$ and $\bar{\psi}_2 = \psi_{2,0}^\dagger = (\bar{\psi}_{2A}, \bar{\psi}_{2B}, \bar{\psi}_{2A}, \bar{\psi}_{2B})$. $\gamma_\mu$ is defined as $\gamma_0 = \sigma_0 \otimes \tau_2$, $\gamma_1 = \sigma_0 \otimes \tau_\gamma$, $\gamma_2 = \sigma_0 \otimes \tau_x$, $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\tau^x$, $\tau^y$, $\tau^z$ are Pauli matrices. We have set the Fermi velocity to be unit $v_F = 1$.

In the strongly coupling limit, $U >> t$, there always exists an AF order in the extended Hubbard models. Introducing Stratonovich-Hubbard fields for the spin degrees of freedom [13], we obtain the partition function as

$$Z = \int \mathcal{D}\sigma \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\frac{1}{\beta} L}$$

where $L = \int \mathcal{D}\sigma \mathcal{D}\psi \mathcal{D}\bar{\psi}$ is given by

$$L = \mathcal{L}_f + \sum_{\sigma} \tilde{c}_\sigma (\partial_\mu - m) c_\sigma + \sum_{i,j,\sigma} t_{ij} \tilde{c}_i \sigma c_j \sigma$$

with Pauli matrices $\sigma = (\sigma^x, \sigma^y, \sigma^z)$. Here $\mathcal{B}_j$ is a vector denoting spin configurations, $\mathcal{B}_j = |B_j| n_j$ where $|B_j| = \phi_0$ represents the value of localized spin moments and $n_j$ is a unit vector describing the Néel order parameter. In AF ordered state, the mass gap of the electrons is given as $m = \phi_0 U$.

Then starting from Eq. (3), we get the same long wavelength effective model of nodal AF insulator [18, 19, 20]

$$L_{eff} = \sum_\alpha i\bar{\psi}_\alpha \gamma_\mu \partial_\mu \psi_\alpha + m(\bar{\psi}_1 n_\sigma \psi_1 - \bar{\psi}_2 n_\sigma \psi_2)$$

$\alpha = 1, 2$ labels the two Fermi points

Zero modes on half skyrmions - In this section we will study the properties of topological solitons. Instead of considering topological solitons with integer topological charge (skyrmions), we focus on solitons with a half topological charge, $\frac{1}{2} \int n_x \cdot \partial_x n_x \otimes \partial_x n_y d^2 r = \pm \frac{1}{2}$ with $r = (x, y)$. Such soliton is called a half skyrmion (meron or antimeron). A meron with a narrow core size (the lattice size $a$) is characterized by $n = r / |r|$, $r^2 = x^2 + y^2 \approx 21, 22, 23, 24, 25, 26, 27, 28$. To stabilize such a solitons, one may add a small easy-plane anisotropy of the Néel order.

Around a meron configuration, the fermionic operators are expanded as

$$\psi_\alpha (r, t) = \sum_{k \neq 0} \hat{b}_{\alpha k} e^{-iE_k t} \psi_{\alpha k} (r)$$

where $\hat{b}_{\alpha k}$ and $\bar{\hat{b}}_{\alpha k}$ are operators of $k \neq 0$ modes that are irrelevant to the soliton states discussed below. $\psi_{\alpha k}^\dagger (r) = (\psi_{\alpha k}^{0 A k}, \psi_{\alpha k}^{0 B k}, \psi_{\alpha k}^{0 A k}, \psi_{\alpha k}^{0 B k})$ are the functions of zero modes. $\bar{\hat{b}}_{\alpha k}$ are annihilation operators of zero modes.

To obtain the zero modes, we write down two Dirac equations from Eq. (5)

$$i\partial_\sigma \gamma_1 \psi_1^0 + i\partial_\sigma \gamma_2 \psi_2^0 + m n_\sigma \psi_1^0 = 0$$

and

$$i\partial_\sigma \gamma_1 \psi_2^0 + i\partial_\sigma \gamma_2 \psi_2^0 - m n_\sigma \psi_2^0 = 0$$

Firstly we solve the Dirac equation for $\psi_1^0$. With the ansatz $\psi_1^0 = (\xi_1(\hat{x} ) e^{-i\theta}, \xi_3(\hat{x} ) e^{i\theta})$, we have

$$\partial_2 \xi_2 = \xi_3, \partial_2 \xi_3 = \xi_2, \partial_2 \xi_4 = -\frac{\xi_4}{x} + \xi_1$$

where $\hat{x} = |r| (\cos \theta, \sin \theta)$ and $x = \frac{r^2}{\beta}$. The solution has been obtained in Ref. [22] as

$$\xi_1(\hat{x} ) = \xi_4(\hat{x} ) = 0, \xi_2(\hat{x} ) = \xi_3(\hat{x} ) = \hat{x} + K_\frac{\beta}{\beta} (\hat{x} )$$

where $K_\frac{\beta}{\beta} (\hat{x} )$ is the modified Bessel function. So the solution of $\psi_1^0$ becomes

$$\begin{pmatrix} 0 \\ \hat{x} + K_\frac{\beta}{\beta} (\hat{x} ) \\ 0 \\ 0 \end{pmatrix}$$

To solve $\psi_2^0$, we transform the equation

$$U i\partial_\sigma \gamma_1 \psi_2^0 U^{-1} + m n_\sigma \psi_2^0 U^{-1} = 0$$

with $U = e^{i\pi \gamma_0 / 2}, U_1 U^{-1} = -\gamma_i$ and $U^{-1} \psi_2^0 U = \tilde{\psi}_2^0$.

Then the solution of $\psi_2^0$ is obtained as

$$\begin{pmatrix} 0 \\ -\hat{x} + K_\frac{\beta}{\beta} (\hat{x} ) \\ \hat{x} + K_\frac{\beta}{\beta} (\hat{x} ) \\ 0 \end{pmatrix}$$

It is noticeable that from above solutions of zero modes, the components $\psi_{1A,1B}^0, \psi_{1A,2A}^0$ and $\psi_{1A,2B}^0$ are all zero. Topological mechanism of spin-charge separation - For the solutions of zero modes, there are four zero-energy soliton states $|sol\rangle$ around a half skyrmion which are denoted by $|1_+\rangle \otimes |2_+\rangle, |1_-\rangle \otimes |2_-\rangle, |1_0\rangle \otimes |2_0\rangle$ and $|1_+\rangle \otimes |2_-\rangle, |1_-\rangle \otimes |2_+\rangle$ are empty states of the zero modes $\psi_1^0 (r)$ and $\psi_2^0 (r)$: $|1_+\rangle$ and $|2_+\rangle$ are occupied states of them. Thus we have the relationship between $\hat{a}_\sigma^0$ and $|sol\rangle$ as

$$\hat{a}_1^0 |1_+\rangle = |1_-\rangle, \hat{a}_0^0 |1_-\rangle = 0, \hat{a}_2^0 |2_+\rangle = |2_0\rangle, \hat{a}_2^0 |2_0\rangle = 0.$$

(12)
Firstly we define total induced fermion number operators of the soliton states, \( \hat{N}_F = \sum_\alpha \hat{N}_\alpha, \hat{F} \) with

\[
\hat{N}_{\alpha,F} \equiv \int : \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha : d^2 r \tag{13}
\]

\[
= (\hat{a}_\alpha^0)^\dagger \hat{a}_\alpha^0 + \sum_{k \neq 0} (\hat{\beta}_\alpha k \hat{\beta}_\alpha k - \hat{a}_\alpha k \hat{a}_\alpha k) - \frac{1}{2}.
\]

\( \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha \) : means normal product of \( \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha \). From the relation between \( \hat{a}_\alpha^0 \) and \( | \text{sol} \rangle \) in Eq.(12), we find that \( | 1_\pm \rangle \) or \( | 2_\pm \rangle \) have eigenvalues of \( \pm \frac{1}{2} \) of the total induced fermion number operator \( \hat{N}_F \),

\[
\hat{N}_{1,F}|1_\pm \rangle = \pm \frac{1}{2}|1_\pm \rangle, \quad \hat{N}_{1,F}|2_\pm \rangle = 0, \tag{14}
\]

\[
\hat{N}_{2,F}|2_\pm \rangle = \pm \frac{1}{2}|2_\pm \rangle, \quad \hat{N}_{2,F}|1_\pm \rangle = 0.
\]

Another important induced quantum number operator is staggered spin operator, \( \hat{S}_{(\pi,\pi)}^z = \frac{1}{2} \sum_{i \in A} \hat{c}_i^\dagger \sigma_z \hat{c}_i \).

Using above four equations, we obtain

\[
\hat{S}_{(\pi,\pi)}^z | \text{sol} \rangle = \frac{1}{2} \int d^2 r : (- \hat{\psi}_{1A}^\dagger \hat{\psi}_{1A} - \hat{\psi}_{1B}^\dagger \hat{\psi}_{1B} - \hat{\psi}_{1A}^\dagger \hat{\psi}_{1A} - \hat{\psi}_{1B}^\dagger \hat{\psi}_{1B}) | \text{sol} \rangle
\]

\[
+ \hat{\psi}_{12A}^\dagger \hat{\psi}_{12A} + \hat{\psi}_{12B}^\dagger \hat{\psi}_{12B} + \hat{\psi}_{12A}^\dagger \hat{\psi}_{12A} + \hat{\psi}_{12B}^\dagger \hat{\psi}_{12B}) | \text{sol} \rangle = \frac{1}{2} (\hat{N}_{1,F} - \hat{N}_{2,F}) | \text{sol} \rangle.
\]

Then we calculate two induced quantum numbers defined above. Without doping, the soliton states of a half skyrmion are denoted by \( | 1_- \rangle \otimes | 2_+ \rangle \) and \( | 1_+ \rangle \otimes | 2_- \rangle \). One can easily check that the total induced fermion number on the solitons is zero from the cancelation effect between two nodals \( \hat{N}_F | 1_- \rangle \otimes | 2_+ \rangle = \hat{N}_F | 1_+ \rangle \otimes | 2_- \rangle = 0 \). It is consistent to the earlier results that forbid a Hopf term for the low energy theory of two dimensional Heisenberg model \([30]\). On the other hand, there exists an induced staggered spin moment on the soliton states \( | 1_- \rangle \otimes | 2_+ \rangle \) and \( | 1_+ \rangle \otimes | 2_- \rangle \),

\[
\hat{S}_{(\pi,\pi)}^z | 1_- \rangle \otimes | 2_+ \rangle = \frac{1}{2} | 1_- \rangle \otimes | 2_+ \rangle, \tag{16}
\]

\[
\hat{S}_{(\pi,\pi)}^z | 1_+ \rangle \otimes | 2_- \rangle = - \frac{1}{2} | 1_+ \rangle \otimes | 2_- \rangle.
\]

The induced staggered spin moment may be straightforwardly obtained by combining the definition of \( \hat{S}_{(\pi,\pi)}^z \) and Eq.(14) together.

When half skyrmions become mobile, their quantum statistics becomes important. Let us examine the statistics of a half skyrmion with an induced staggered spin moment. In CP(1) representation of \( n \), a "bosonic spinon" is introduced by \( n = \bar{z} z \) with \( z = \left( \begin{array}{c} z_1^\dagger \\ z_2 \end{array} \right) \) and \( \bar{z} z = 1 \). Since each "bosonic spinon" \( z \) carries \( \pm \frac{1}{2} \) staggered spin moment, an induced staggered spin moment corresponds to a trapped "bosonic spinon" \( z \). On the other hand, a half skyrmion can be regarded as a \( \pi \) flux of the "bosonic spinon", \( \int \frac{2 \pi}{\hbar} \bar{n} \cdot \partial_z n \times \partial_y n \) \( d^2 r = \frac{\pi}{\hbar} \int \epsilon_{\mu\nu}\partial_\mu a_\nu d^2 r = \pm \frac{1}{\hbar} \) with \( a_\mu \equiv \frac{\pi}{\hbar} (\hat{\alpha}_{\mu} z - \hat{\beta}_{\mu} \bar{z} z) \). To be more explicit, moving a "bosonic spinon" \( z \) around a half skyrmion generates a Berry phase \( \phi \) to \( z \rightarrow z' = \left( \begin{array}{c} z_1 e^{i\phi} \\ z_2 e^{i\phi} \end{array} \right) \) where \( \phi = \int \epsilon_{\mu\nu}\partial_\mu a_\nu d^2 r = \pm \pi \). As a result, a "bosonic spinon" \( z \) and a half skyrmion (meron or antimeron) share mutual semion statistics. Binding the trapped "bosonic spinon", a mobile half skyrmion becomes a fermionic particle. We may use the operator \( f_\sigma \) to describe such neutral fermionic particle with half spin. The relation between the zero energy states and the fermionic states is given as \( | 1_+ \rangle \otimes | 2_- \rangle = f_+^\dagger | 0 \rangle \) and \( | 1_- \rangle \otimes | 2_+ \rangle = f_-^\dagger | 0 \rangle \) (The state \( | 0 \rangle \) is defined through \( f_+^\dagger | 0 \rangle = f_+^\dagger | 0 \rangle = 0 \). We call such neutral object (fermion with \( \pm \frac{1}{2} \) spin degree freedom) a (fermionic) "spinon".)

Now we go away from half filling. It is known that when a hole (electron) is doped, it is equivalence to removing (adding) an electron. Without considering the
existence of half skyrmions, the hole (electron) will be doped into the lower (upper) Hubbard band. The existence of zero modes on half skyrmions leads to the appearance of bound levels in the middle of the Mott-Hubbard gap. The hole (electron) will be doped onto the bound states on the half skyrmion and then one of the zero modes is occupied. When one hole is doped, the soliton state is denoted by $|\uparrow\rangle \otimes |2\rangle$. One can easily check the result by calculating its induced quantum numbers. On the one hand, there is no induced staggered spin moment, $S^{z}_{(\pi,\pi)} |1\rangle \otimes |2\rangle = 0$. On the other hand, the total fermion number is not zero, $\hat{N}_{F}|1\rangle \otimes |2\rangle = -|1\rangle \otimes |2\rangle$. These results mean that such soliton state is a spinless "holon" with positive charge degrees of freedom. After binding a fermionic hole, the soliton state (holon) does not have an induced staggered spin moment. Thus the holon obeys bosonic statistics and becomes a charged bosonic particles. When one electron is doped, the soliton state is denoted by $|\uparrow\rangle \otimes |2\rangle$. The induced quantum numbers of it are $\hat{N}_{F}|1\rangle \otimes |2\rangle = +|1\rangle \otimes |2\rangle$ and $S^{z}_{(\pi,\pi)} |1\rangle \otimes |2\rangle = 0$. Such soliton state is also a bosonic particle with a negative charge but without spin degrees of freedom. We call such a soliton state an "electron" to mark difference with the word "electron".

Finally we get a topological mechanism of spin-charge separation in nodal AF insulators. There exist two types of topological objects - one is the fermionic spinon, the other is the bosonic holon (or the bosonic electron).

In 1D system, real spin-charge separation may occur. As far as the low energy physics is concerned, the spin and charge dynamics are completely decoupled from each other. In 2D, real spin-charge separation in a nodal AF insulators can not occur in long range AF order. In the future we will study the deconfinement condition of spin-charge separated solitons and explore the properties of deconfined phases with real spin-charge separation.

Summary - By using 2D $\pi$-flux phase Hubbard model and the Hubbard model on a honeycomb lattice as examples, we explore spin-charge separation in nodal AF insulator. The crus crux of the matter in this paper is the discovery of induced staggered spin moment $S^{z}_{(\pi,\pi)}$ on half skyrmions in nodal AF insulators. Based on such nontrivial induced quantum number, we classify four degenerate soliton states with zero energy - two of them ($|\downarrow\rangle \otimes |2\rangle$ and $|\uparrow\rangle \otimes |2\rangle$) represent the up-spin and down-spin states for a fermionic "spinon", another state ($|1\rangle \otimes |2\rangle$) represents a "holon" and the last one ($|\downarrow\rangle \otimes |2\rangle$) denotes an "electron".

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| $N_{F}$ | $S^{z}_{(\pi,\pi)}$ |
|--------|----------------|
| 1      | 0              |
| 0      | 1/2            |
| 0      | -1/2           |
| -1     | 0              |

TABLE I: Quantum numbers of the degenerate soliton states.

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