Detection of pairing from the extended Aharonov-Bohm period in strongly correlated electron systems

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Abstract

Inspired from Sutherland’s work [Phys. Rev. Lett. 74, 816 (1995)] on detecting bound spin waves, we propose that bound electron states can be detected from the dependence of interacting electron systems to the Aharonov-Bohm flux in the ‘extended zone’ scheme, where the electron pairing halves the original period $N_a$ flux quanta in a system of linear size $N_a$. Along with the Bethe-ansatz analysis, a numerical implementation for keeping track of the adiabatic flow of energy levels is applied to the attractive/repulsive Hubbard models and the $t-J$ ladder.

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The response to an adiabatic change against external parameters is an interesting way to probe the nature of interacting electron systems. Some thirty years ago, Byers and Yang [1] proposed a notable example of detecting the Cooper pairing: while a normal state responds to an Aharonov-Bohm (AB) flux periodically with the period of flux quantum, $\Phi_0 \equiv \hbar c/e$, a BCS state will have a halved period, $\Phi_0/2$. The anomalous flux quantization has actually been applied to various strongly correlated electron systems that are intended to describe high-$T_c$ cuprates [2–5].

This is in fact one out of several ways to detect superconductivity in purely electronic systems. Since an effective electron-electron attraction per se does not guarantee the Cooper pairing, a usual way is to search for a long-tailed pairing correlation function, but the finite-size effect must be carefully analyzed. The quantum Monte Carlo method (QMC) [6–8], the density-matrix renormalization group [9], evaluation of the superfluid density (helicity modulus) [10,4] are toward this line of approach. Thus the detection of the Cooper pairing (or bound electrons in more general terms) is a demanding problem in a correlated electron gas, except for one-dimensional (1D) systems, where exact analytic treatment is feasible with the Bethe-ansatz solutions coupled with the conformal field theory.

This is where the Byers-Yang flux quantization comes in. The test, however, remains some way from a clear-cut criterion, since the flux dependence of the ground-state energy may give the half-flux periodicity even for the repulsive Hubbard model [3]. An origin of the obscured period is the spin degrees of freedom [11], which is most prominent in 1D.

In the present paper, we propose a new way to detect bound electron states from a more global look at the response to the flux. The idea has been inspired by a recent analysis of the bound spin waves by Sutherland [12]: bound complexes of spin waves in 1D Heisenberg magnets (or equivalently a gas of charged bosons) may be detected from their response to a boosted total momentum. The momentum boost is achieved by twisting the boundary condition, $\Psi(\ldots, x_j + N_a, \ldots) = e^{i2\pi\phi}\Psi(\ldots, x_j, \ldots)$, for an $N_a$-site lattice, which uniformly shifts the set of $k$ points. He has shown that, if all of the $N$ particles (i.e., $N$ flipped spins in a magnet) form one bound state, the energy returns to its initial value by a twist of
\( \phi = N_a/N \), which is \( 1/N \) times the twist \( \phi = N_a \) required to shift the set of \( k \) points for the free particles back to the original position. Intuitively, this discerns whether the momentum boost acts on individual particles or on a ‘center-of-mass’ of bound particles. A key in Sutherland’s idea is to keep track of the \( \phi \)-dependence of the state not over the one period \((0 \leq \phi < 1)\) but over the ‘extended zone’ \((0 \leq \phi < N_a)\).

Sutherland does not argue what happens in electron systems or in the situation where more than one bound complexes exist, but we conjecture here that the extended AB method should, conceptually, hold in general. We would then be able to treat \( e.g. \) the Cooper pairing problem. Natural questions are: (i) Can we really extend Sutherland’s spin-wave analysis to electron systems? (ii) Can we apply the method to two or higher dimensions?

In the present Letter we first give a straightforward extension of Sutherland’s spin analysis to electron systems with the Bethe-ansatz analysis of the 1D Hubbard model as a prototype. There we introduce an AB flux \( \Phi \) that couples to the charge degrees of freedom to twist the boundary condition. We then look at the energy levels against \( \Phi \) over \( 0 \leq \Phi < N_a \Phi_0 \) (which we call the ‘extended AB’ spectral flow) to discriminate the bound states, as opposed to the conventional wisdom that one period of \( \Phi_0 \) suffices. We next propose a method to numerically implement the extended AB test for arbitrary systems including 2D systems to go beyond the Bethe-ansatz analysis.

We start with confirming for the 1D Hubbard model that the electrons have a reduced period of \( N_a \Phi_0/N \) as well for \( N \)-bound states with the Bethe-ansatz analysis \[13\]. Consider an \( N_a \)-site ring (with \( N_a \) even for simplicity) containing \( N \) electrons, and thread a magnetic flux \( \Phi \). A change of \( \Phi \) by \( \Phi_0 \) shifts the \( k \) points exactly by their spacing \( \Delta k = 2\pi/N_a \) for noninteracting electrons, so that the set of \( k \) points accomplishes a full travel across the Brillouin zone when \( \Phi/\Phi_0 \) reaches \( N_a \). When interacting, the electrons are subject to Bethe-ansatz equations \[14\], for which there are two types of solutions, i.e., real and complex roots \[15\]. A real charge rapidity \( k_j \) represents the quasi-momentum of a beam of charges, while complex \( k_j \)'s, which are sometimes called string solutions because they appear in a linear group with a common real part, represent bound states of electrons.
For a set of real \( k_j \)'s, we can take a logarithm of Bethe-ansatz equations to have

\[
k_j N_a = 2\pi I_j + 2\pi \Phi/\Phi_0 - \sum_{\alpha=1}^{M} 2\tan^{-1}\frac{4}{U} (\sin k_j - \Lambda_{\alpha}),
\]

(1)

where \( M \) is the number of down spins, \( t \) the transfer, \( U \) the Hubbard interaction, and \( I_j \) \((j = 1, \ldots, N)\) is an integer (half odd integer) for an even (odd) \( M \). We assume that spin rapidities \( \Lambda_{\alpha} \) are real as is the case with the ground state of the repulsive model. Equation (1) has a periodicity of \( N_a \) in \( I_j \). Since an increase of \( \Phi \) by \( \Phi_0 \) causes a uniform shift of \( I_j \) by unity, a real solution indeed has a periodicity of \( N_a \Phi_0 \) (except at the half-filling, see below).

Now, the string solutions for charge rapidities, \( \{k_{nl} \ (l = 1, \ldots, 2n)\} \), are specified by a single real parameter, \( \Lambda'_{n} \) [13]. When all the \( N \) particles form a single bound state (an \( N \)-bound state in Sutherland’s words), the equation reduces to

\[
\exp(iN_a \sum_{l} k_{nl}) = \\
\exp\left\{-iN_a[\sin^{-1}(\Lambda'_{n} + inU/4) + \sin^{-1}(\Lambda'_{n} - inU/4)]\right\} = \exp(i2\pi N\Phi/\Phi_0).
\]

(2)

We can then see that \( \Lambda'_{n} \) is determined by the total momentum \( \sum_{l} k_{nl} \), so that a change of \( \Phi \) by \( \Phi_0/N \) is enough to shift \( \Lambda'_{n} \) to the next position among the \( N_a \) solutions. Thus we end up with a period of \( N_a \Phi_0/N \) for a single \( N \)-bound state.

Solutions having more than one set of strings have been known to exist for e.g., the attractive Hubbard model having a set of two-strings (electron pairs) [16,17]. However, their high-energy spectra has not been fully understood, so that the spectral flow has to be obtained numerically even in 1D.

So we move on to the numerical implementation of looking at the flow, which is readily applicable to two or higher spatial dimensions, and also to various models such as the extended Hubbard or \( t-J \) models. In determining the extended period, we have to keep track of the ground state for the range of the flux well beyond the flux quantum, where the energy level soars to become high-energy states. In addition the level has to be traced straight through level crossings, so that the numerical method must be good enough to
reproduce (a) level crossings and (b) high-energy states. Conventional methods such as the exact diagonalization or quantum Monte Carlo methods would then be inadequate.

The algorithm we propose consists of successive estimations of the energy and wave function for $\Phi + \Delta \Phi$. The new state $\Psi$ is estimated by multiplying a connection, $e^{iA(\Phi)\Delta \Phi}$, defined as

$$\Psi(\Phi + \Delta \Phi) = e^{iA(\Phi)\Delta \Phi} \Psi(\Phi).$$  \hspace{1cm} (3)

Here a matrix $A$ is approximately diagonal ($e^{iA_i \Delta \Phi} \approx \Psi_i(\Phi + \Delta \Phi)/\Psi_i(\Phi)$) for a small enough $\Delta \Phi$, where $\Psi_i$ denotes the $i$-th component. Namely the connection reduces to a set of pure phases (i.e., Berry’s geometrical phase). Each estimation is followed by a correction in the following recursive manner.

i) Start from the ground state $\Psi(\Phi = 0)$ and the next one $\Psi(\Delta \Phi)$ which are obtained by the Lanczos method.

ii) Predict the connection from the previous step as $e^{iA_i \Delta \Phi} \approx \Psi_i(\Phi)/\Psi_i(\Phi - \Delta \Phi)$ to produce the next one, $\tilde{\Psi}(\Phi + \Delta \Phi) = e^{iA(\Phi)\Delta \Phi} \Psi(\Phi)$.

iii) Correct $\tilde{\Psi}$ by operating some power, $m$, of the resolvent as

$$\left\{ \frac{1}{[H(\Phi + \Delta \Phi) - E]^2} \right\}^m \tilde{\Psi}(\Phi + \Delta \Phi) \xrightarrow{m \to \infty} \Psi(\Phi + \Delta \Phi).$$  \hspace{1cm} (4)

This power method is performed with the inverse-iteration and the conjugate-gradient optimization. $E$ in the resolvent can be calculated accurately from the wavefunction updated every time we increase $m$.

iv) Check the convergence, $|(H(\Phi + \Delta \Phi) - E)\Psi(\Phi + \Delta \Phi)| < \varepsilon$, for a given accuracy $\varepsilon$. Increase $m$ until this inequality is fulfilled, then move on to ii).

Applied over the extended zone, the method can count the periodicity (or the ‘winding number’) of the state. The tractable matrix size is the similar to that for the conventional Lanczos diagonalization.

Around level crossings the calculation becomes subtle. We first observe that level crossings come in two classes: One class occurs for two levels that differ in some symmetry of
the system. The second occurs at a phase transition point, *e.g.*, the normal-superconductor transition. The first class can be dealt with by only letting the convergence criterion in iv) with typically $\varepsilon = 10^{-8}$ for the systems considered here with the matrix size up to a few ten thousands. The second class requires scaling analysis by varying the distance from the critical point as illustrated for the $t - J$ ladder below.

Our first example is the 1D Hubbard model. Figure 1 compares the spectral flow for a 10-site ring with 6 electrons for a repulsive model with $U/t = +1$ and an attractive model with $U/t = -1$. The extended period, which is $N_\alpha \Phi_0$ for the repulsive model, is indeed halved for the attractive case, providing a clear-cut detection of the two-electron pairing.

For comparison, we have superposed the anomalous flux quantization test for $0 \leq \Phi < \Phi_0$ in Fig.1. We can see that the latter test is indeed ambiguous. To be more precise, we can observe the following. If the Fermi sea has a closed shell ($N \equiv 2 \mod 4$, as is the case with Fig.1), the true ground state is always spin singlet irrespective of the sign of $U$. In addition to the branch starting from the ground state, there is a second branch, which is degenerate with the first one at $\Phi = \Phi_0/2$ for $U = 0$ but shifts upward for a repulsive interaction, or downward for an attractive interaction. Thus a dip appears in a continuous fashion as a negative $U$ is turned on. However, the half periodicity can appear even for the repulsive interactions for open-shell Fermi seas [3]. This is due to the existence of a spin-triplet state, which is degenerate with the ground state at $\Phi = 0$ and stabilized over the singlet state for $U > 0$ [18]. If we further go into the strong correlation limit, even more anomalous $1/N_e$-periodicity can appear as shown by Kusmartsev [11]. Thus we have to worry about these finite-size effects due to other branches lying around to obscure the period in the anomalous flux quantization. In two or higher dimensions such situations may be improved [10,5], but we should re-emphasize that the winding-number counting here concentrates on the adiabatic evolution of a *single* state, where the ‘global’ period is determined independently of other branches.

The abrupt change from $N_\alpha \Phi_0$ to $N_\alpha \Phi_0/2$ in the extended AB period takes place exactly at $U = 0$, which is the critical point in 1D. The change occurs despite the fact that three
spectral flows (for $U < 0, U = 0, U > 0$) are almost identical around the respective minimum except for some offsets. This corresponds to the known fact [10] that the charge stiffness (or Drude weight) does not exhibit singular jumps even at the critical point when the system is finite.

A closer inspection shows that the long AB period for $U \neq 0$ is dominated by some level crossings that turn into a level repulsion or level *anticrossings*, where different sets of anticrossings are selected according as $U > 0$ or $U < 0$. It is at first puzzling how such a qualitative change can possibly occur for an infinitesimal $|U|$, since charge rapidity $k_j$'s coalesce into doubly occupied $k$ points in the Fermi sea no matter how the critical point ($U = 0$) is approached from repulsive or attractive sides (see Ref. [19]).

The puzzle is resolved by looking at the weak-coupling Bethe-ansatz behavior. As the $k$ points shift with $\Phi$, the crucial level anticrossing occurs when the upper-most doubly-occupied $k$ point reaches $k_0 = \pi/2$ situated at $\varepsilon(k_0) = 0$, the center of the band dispersion. This special point accommodates highly degenerate states that are connected by two-particle scattering processes that comprise the normal ones, $c_{k_0\uparrow}^\dagger c_{k_0\downarrow}^\dagger \rightarrow c_{k_0+p\uparrow}^\dagger c_{k_0-p\downarrow}^\dagger$, with $p$ the momentum transfer, along with the Umklapp process, $c_{k_0\uparrow}^\dagger c_{k_0\downarrow}^\dagger \rightarrow c_{k-2k_0\uparrow}^\dagger c_{k-2k_0\downarrow}^\dagger$. When $U$ is switched on, the degenerate perturbation dictates that some of these states must mix to give anticrossings.

The normal process with $p = 2\pi N/N_a$ selectively produces the anticrossing for the repulsive case. In contrast, the anticrossing in the attractive case is caused by the Umklapp process that transfers a pair to other $\varepsilon = 0$ points, which is the only possible process indeed if the pairs are not dissociated by the adiabatic change in $\Phi$. The fact that $k_0$ is the key position is illustrated in Fig.1: it takes $\Phi_c/\Phi_0 = (k_0 - k_F)/\Delta k$ for the upper-most doubly occupied $k$ point ($k_F$) to reach $k_0$, where $\Phi_c/\Phi_0 = 1.5$ for $N_e = 6, N = 10$, in exact agreement with Fig.1.

Given this property, we can readily show that a series of dissociations of doubly occupied states for $U > 0$ gives the extended period of $N_a \Phi_0$, while a series of Umklapped doubly occupied states for $U < 0$ halves it. Thus, an infinitesimal interaction is enough to change
the global topology (the winding number) of the connection in this example in 1D.

A fuller understanding in terms of the spin-charge separation in 1D emerges if we look more closely at the Bethe ansatz, where $\Lambda_\alpha$ (a ‘spin degrees of freedom’), not directly coupled with $\Phi$, stays approximately constant, while the ‘charge degrees of freedom’ $k_i$ progressively changes with $\Phi$ for a repulsive $U$. This is accomplished by $\Lambda_\alpha$ sequentially parting company with one $k_i$ to meet another, which is exactly where the anticrossings occur. On the other hand, each $\Lambda_\alpha$ is attached to a pair, $k_j, k_j^*$, for an attractive $U$, and the center-of-mass momentum, $2\text{Re}(k_j)$, of the pair remains within the first Brillouin zone due to the Umklapp process, or equivalently, $k_j$’s have to satisfy $\cos(k_j) \geq 0$ for the two-bound solutions to exist. The details will be published elsewhere.

In order to demonstrate that the present method is applicable to the case in which the Bethe-ansatz is inapplicable, and also to provide a step toward higher dimensions, we move on to the $t$-$J$ ladder model. This model, originally conceived for some copper or vanadium oxides, is believed to exhibit superconductivity for small hole doping from the half-filling $[20]$. Here we perform the extended AB test for a $6 \times 2$-site system with 4 electrons, which corresponds to a hole concentration of $n = 2/3$.

In the result, Fig.2, we can clearly see that the periodicity is halved into $N_a/2$ as $J$ is increased to $J > 2.04t$, which indicates paring. Here we can illustrate a nice feature about the extended AB test: since the transition is associated with a level crossing (a cusp) turning into an anticrossing, we can numerically plot (inset of Fig.2) the size, $\Delta$, of the level repulsion against the relevant parameter ($J$ here) to identify the critical point ($J_c \simeq 2.04$ here) at which $\Delta$ vanishes. Thus we can estimate the critical value $J_c$ for a finite system in a well-defined manner, which may then be cast into a finite-size scaling analysis for a more pertinent definition of the critical point. Thus the present method provides a possible way to determine the phase diagram of a given model.

So far we have not discussed anything directly about the coherence of the pairs, so that we are talking about a necessary condition for superconductivity. For that matter, Byers-Yang theorem also gives a necessary condition for the superconductivity (or the Meissner
effect). It is an intriguing future problem to see if the coherence can possibly appear in the spectral flow.

Another comment is that the present test gives information on metal-insulator transitions such as the Mott-Hubbard transition as well. For the half-filled Hubbard model (a Mott’s insulator), the extended AB period reduces down to $\Phi_0$. The sudden change from the full period $N_0 \Phi_0$ to the minimum one is due to an appearance of the charge gap, across which the flow is inhibited to jump so that the system has to return to the original state as soon as the flux reaches $\Phi_0$, in analogy with the gauge argument of the quantum Hall effect. Thus we can expect that the present method can detect the existence or otherwise of the Fermi surface [21]. A more interesting example is the phase separation, where the system should respond as a single bound state as will be reported elsewhere. The different winding numbers for paired, metallic and insulating phases may be analyzed in terms of the homotopy of the phase-space (or the fiber bundle) of correlated electron systems.

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FIGURES

FIG. 1. The result for the spectral flow for a 10-site Hubbard ring with 6 electrons. The flow
lines represent a repulsive case \( U = t \), a solid line), an attractive case \( U = -t \), a dashed line), and
the non-interacting case (dotted line). The relevant level crossing point is marked with \( \Phi_c \). For
comparison, the low-lying flows over one period of the flux quantum is reproduced.

FIG. 2. The spectral flow lines for a \( t-J \) ladder model with 4 electrons in \( 6 \times 2 \) sites for
\( J = 2.2, 2.6, \ldots, 3.8 \) from top to bottom. The inset depicts the size, \( \Delta \), of the relevant level
repulsion against \( J \), where the line is a guide to the eye.