Breakdown of electron-pairs in the presence of an electric field of a superconducting ring

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Abstract

The quantum dynamics of quasi-one-dimensional ring with varying electron filling factors is investigated in the presence of an external electric field. The system is modeled within a Hubbard Hamiltonian with attractive Coulomb correlation, which results in a superconducting ground state when away from half-filling. The electric field is induced by applying time-dependent Aharonov–Bohm flux in the perpendicular direction. To explore the non-equilibrium phenomena arising from the field, we adopt exact diagonalization and the Crank–Nicolson numerical method. With an increase in electric field strength, the electron pairs, a signature of the superconducting phase, start breaking and the system enters into a metallic phase. However, the strength of the electric field for this quantum phase transition depends on the electronic correlation. This phenomenon has been confirmed by flux-quantization of time-dependent current and pair correlation functions.

Keywords: superconducting ring, time-dependent Aharonov–Bohm flux, exact diagonalization and Crank–Nicolson

(Some figures may appear in colour only in the online journal)

1. Introduction

The strongly correlated low-dimensional systems and their response to the external perturbations, e.g. applied fields, has been an ever-growing research area owing to their rich quantum phase diagram. Recent advancements in experiments enable the realization of the quantum dynamics in materials [1–4] and in the cold atom system [5–8] in the non-equilibrium environment. Dielectric breakdown of the Mott insulating phase in organic thyristor [3] and one-dimensional systems, such as, Sr₂CuO₃ and SrCuO₂ [4] has been realized experimentally in the presence of strong electric fields. There has been a report of photo-induced Mott transition in a halogen-bridged Ni-chain compound as well [1]. In cold atom systems, such as one-dimensional Bose gases, the non-equilibrium dynamics of superfluids has been studied [6]. Three-dimensional fermionic optical lattices also exhibit band-insulator to metal transition by controlling the interaction between atoms through the Feshbach resonance [8].

In a recent experiment, the breaking of electron-pairs, namely Cooper-pairs of a superconducting system, is shown by exposing it to photon flux [14]. At a low enough temperature, superconductors are a condensate of Cooper-pairs which are sensitive towards the external perturbations. Motivated by these experiments, here we study the breaking of electron pairs in superconducting rings, which can be realized experimentally [9, 10] along with the measurement of their persistent current [11–13]. The superconducting rings are described by the attractive Hubbard model. Here the net effective attractive interaction forms the electron pairs, leading to superconductivity [16–18]. In the real materials, the origin of this attractive interaction can also be due to the coupling between the electron and lattice, excitons or plasmons [19]. For lower values of attractive interaction, electrons form BCS (Bardeen–Cooper–Schrieffer) type of pairing with loosely bound pairs, but increase in attractive interaction results in strong local pairing (BEC-limit (Bose–Einstein condensate)) [20]. These strong-pairs that are similar to charged bosons...
can condensate and give rise to superconducting states [19].
Therefore, superconductivity requires the formation of electron pairs and phase-coherence between the pairs.

An external electric field induces fluctuation in these pairs and eventually breaks them. We have modeled the external electric field in terms of time-dependent Aharonov–Bohm (AB) flux and studied the non-equilibrium properties and time evolution of the many body wave function by using exact diagonalization and the Crank–Nicolson method. We found that the breaking of electron-pairs depends on the strength of the electric field and attractive interaction. We analyze this depairing of electrons by flux-quantization of the persistent-current, time average current and pair-correlation function.

The flux quantization [21, 22] and the off-diagonal long-range order [23] are the key characteristics of superconductors. The quantization of AB-flux has been observed experimentally in conventional [24, 25] and in high-temperature superconductors [26]. For the free electron system, the quantized flux is \( \phi_0 = \hbar e / f \) [27]. In the case of superconductors, the electron-pairing results in a halved period, i.e. \( \phi = \phi_0 / 2 \) [21, 22, 28–31]. Similar phenomenon can be observed in the case of the repulsive Hubbard model for finite size rings due to the spin degrees of freedom [32], even without superconductivity. This ambiguity has driven us to choose the more global approach of the extended-AB period method to detect the electron-pairing [18, 33, 34], since this keeps track of the evolution of energy levels and the wavefunction as a function of the flux over the extended-AB period we refer to [34]). But whenever there is a formation of the density wave (charge or spin), this periodicity gets confined within the lattice constant, i.e. \( \phi_0 \).

2. Model and numerical method

To investigate the behavior of these electron-pairs in the presence of an external electric field, we considered the quasi-one-dimensional ring structure (see figure 1(a)) and modeled the system within the attractive Hubbard model,

\[
H(t) = -\gamma \sum_{i,\sigma} \exp\left[\frac{2\pi i (t / N) \phi}{\hbar}\right] c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{h.c.} - U \sum_i n_i \sigma n_i \sigma
\]

(1)

where \( \gamma \) and \( U \) are the hopping term and the attractive onsite Coulomb potential. \( c_{i,\sigma}^\dagger \) (\( c_{i,\sigma} \)) creates (annihilates) one electron with spin \( \sigma \) at \( i \)th site and \( n_i \) is the number operator. The electric field \( F \) has been included in terms of time-dependent AB-flux, \( \phi(t) = eFLt \) (see figure 1(a)), \( N = L / a \) denoting the number of sites, \( a \) is the lattice constant and \( t \) being the time. We set \( e = h = a = 1 \) and assume \( \gamma \) as the unit of energy throughout the paper. Since, \( a = 1 \), \( L \) has been considered to be the same as \( N \) in the following sections.

We consider different system lengths \((L = 8, 10 \text{ and } 12)\), with various filling factors \( f \) (\( f = n_e / L \)), where \( n_e \) is the number of electrons in the system). Note that we always consider the same number of up and down spins to keep the \( z \)-component of the total spin, \( s_z^{\text{total}} \) as zero. In the absence of an electric field, the above model results in a superconducting ground state [15–19], but away from half-filling. However, at half-filling the superconducting state becomes degenerate with a charge density wave ground state. At half-filling, a large enough negative value of \( |U| \) ensures the pairing of electrons at alternate sites. Therefore, the ground state becomes alternate bound pairs and empty sites, which constitutes a charge density wave (charge or spin), this periodicity gets confined within the lattice constant, i.e. \( \phi_0 \).

Figure 1. (a) The schematic of a quasi-one-dimensional ring with 12 sites. The time dependent perpendicular AB flux, \( \phi(t) \) generates the circulating electric field, \( F \) in the ring. (b) Time evolution of the non-interacting \((U = 0)\) ground state energy \( E \), as a function of \( \phi(t) / \phi_0 \), for \( F = 0.0005 \) with varying filling factors \( f \).
ψ(t + δt)⟩ = \exp^{-i \int_0^\infty \mathcal{H}(\phi(t)) dt} |ψ(t)⟩ \approx \frac{1 - i \frac{\hbar}{\gamma} H(t + \frac{\hbar}{\gamma})}{1 + \frac{i}{2} \hbar \gamma} |ψ(t)⟩ \quad (2)

For precise convergence of the wave-function, the time step \( \delta t \) has been considered to be small enough, 0.01 in units of \( \hbar / \gamma \). This unit of time has been chosen to make the exponential dimensionless. Note that each time evolution step requires the computationally expensive matrix inversion of the many body Hamiltonian matrix. We adopt the Davidson algorithm for this purpose, which gives proper convergence.

**3. Results and discussion**

First we investigate the flux quantization of the ground state energy and the current density as a response to the applied AB-flux with varying filling factor, \( f \) and attractive potential. Then the effect of the electric field on the ground state has been studied to detect the superconducting to metallic phase transition. This has been characterized by further calculations on the pair correlation function and the time averaged current.

In figure 2, we show the time evolution of the ground state energy for the interacting case, as a function of AB-flux for very small \( F \). As can be seen, for non-interacting systems (figure 1(b)), the periodicity is always equal to the extended AB-period, \( L\phi_0 \). Once the attractive interaction is turned on, the periodicity becomes halved, i.e. \( \frac{L\phi_0}{2} \) in the case of smaller \( f \) values (figure 2(a)), indicating the superconducting ground state with the formation of electron-pairs. However, an increase in \( f \) results in additional cusps, coexisting with the halved extended AB-period (figures 2(b) and (c)). These cusps are the signature of level anti-crossings, arising from the enhanced degeneracy in the system with a higher number of electrons [18, 34]. These degenerate states are connected via two-particle scattering processes along with the Umklapp processes [34]. Once the system attains half-filling ( \( f = 1 \) ), the periodicity reduces to \( \phi_0 \) (figure 2(d)), as the system forms the charge density wave phase, with the pairing up of two electrons with opposite spins at alternate sites under the influence of attractive \( U \) [34, 35].

For further characterization of flux quantization, we investigate the current density as a function of the applied AB-flux. The current density operator is defined as.

\[
J(t) = -\gamma \sum_{i, \sigma} i (\exp^{2\pi i \phi(t) / N} c_{i+1, \sigma} c_{i, \sigma}^\dagger - \text{h.c.}) \quad (3)
\]

In figure 3, we show the time evolution of current density as a function of \( \phi(t) = FLt \). Note that the current density is the change in the slope of energy with respect to the flux. Therefore, one can find direct correspondence between the energy and the current density plots as a function of flux (see figures 2 and 3). As expected, the \( \langle J(t) \rangle \) shows the extended AB-period for the non-interacting system. The fractional periodicity [37, 38] in the current (see figures 3(b) and (c)) corresponds to the cusps of energy. The coexistence of the superconducting state, characterized by the halved period and the fractional periodicity can also be seen from \( \langle J(t) \rangle \) plot for \( f < 1 \). Note that, due to the finiteness of the one-dimensional system, the kinetic energy of the electron-pairs tries to break the pairing and leads to the formation of fractional periodicity. Therefore, an increase in the system length or the increase in attractive potential, \( U \) can lead to a stable superconducting ground state with improved half-periodicity [36]. This behavior is clearly visible from the \( U \) dependence of the current density in figure 3.

Furthermore, we systematically increase the system size for a fixed number of electrons, \( n_e = 6 \) and fixed \( U = 2.0 \) and show the current density in figure 4. As can be seen, with a gradual increase in system size from 8 to 10 to 12, the halved periodicity becomes smoother and the fractional periodicities gradually disappear [36].
Next, we investigate the effect of an electric field on the ground state of the superconducting ring consisting of 12 sites with filling factors \( f = 1/3 \) and \( 1/2 \). In figure 5, we show the current density as a function of \( \phi(t) / \phi_0 \) for different values of attractive potential, \( U \) and strength of electric field, \( F \). As can be seen in figure 5(a), the superconducting ground state (characterized by a halved extended AB-period) undergoes the transition to the metallic phase (characterized by the extended AB-period) even in the case of a weak electric field. This is due to the fact that the presence of weak \( U \) forms loosely bound electron pairs which can easily be broken. However, the gradual increase in \( U \) strengthens the electron-pairs and the system requires a stronger electric field for the superconducting to metallic phase transition (see figures 5(b)–(d)). The fractional periodicities also disappear, owing to the fact that the applied electric field closes up the gaps at level anti-crossings, allowing the spectral flow.

For further characterization of this phase transition, we investigate the time evolution of the pair-correlation function as follows [39],

\[
P(r) = \langle c_{i}^\dagger c_{i}^\dagger c_{r} c_{r}\rangle - \langle c_{i}^\dagger c_{r}\rangle \langle c_{i}^\dagger c_{r}\rangle \tag{4}\]

First we have calculated the pair-correlation function \( P(r) \), for the static case (\( \phi = 0 \)). In figure 6 we have shown the plot of \( P(r) \) as a function of \( r \) for different values of \( U \) and different filling factors. We have calculated \( P(r) \) for 12 sites of the fermionic ring, but due to a periodic boundary condition we have shown \( P(r) \) only for 6 sites. It is known that the quasi-long range order of the pair-correlation function is indicative of the superconducting phase at low-dimension [39]. As shown in the figure 6, values of \( P(r) \) increase with attractive interaction \( U \), which indicates the formation of strong electron bound pairs and an increase in phase-coherence within pairs. On the other hand, in the metallic case, it takes either zero or very small nonzero values.

We present the expectation value of pair-correlation, \( \langle P(r) \rangle \) as a function of distance \( r \) and AB flux, \( \phi(t) \) in figure 7 for two different electric field strengths, e.g. \( F = 0.0005 \) and 0.5 and for different filling factors. In the presence of a weak electric field, \( \langle P(r) \rangle \) shows periodic behavior (see the top panel of figure 7) with short-range order corresponding to the energy
maxima at a quarter of the extended AB-period. This may occur due to the loss of phase coherence between the bound pairs and subsequent diminished superconductivity at those flux values. However, the long-range order persists even at a large time regime, showing the existence of the superconducting phase. On the contrary, in the presence of a strong electric field, the \( P(\phi(t)) \) approaches to zero at higher \( \phi(t) = FL/4 \) values (see bottom panel of figure 7), indicating the breakage of Cooper-pairs. This proves the superconducting to metallic phase transition. Note that the value of \( P(\phi(t)) \) does not go to its ideal value of zero due to the probable finite size effect.

To gain further insight, we calculate the time-averaged current as follows [40],

\[
\langle J \rangle = \frac{1}{T} \int_0^T \langle J(t) \rangle dt
\]  

with integration over quarter of the extended AB period \( \phi(t) = L/4 \) and plot that as a function of \( FL \) in figure 8. As we have discussed before, the increase in the applied electric field breaks the electron-pairs and that can cause the increase in the induced current. As can be seen from figures 8(a) and (b), at lower values of \( FL \), the induced current does not increase initially. However, beyond a certain critical strength of \( FL \), the \( \langle J \rangle \) starts increasing. The critical value of \( FL \) increases with the increase in the strength of the attractive potential, \( U \). That necessitates the application of stronger \( FL \) to trigger the superconducting to metallic phase transition. Note that at a higher \( FL \) regime, the \( \langle J \rangle \) gets saturated mainly depending on the available conduction electrons. All these observations are consistent for different filling factors.

### Figure 7
Contour plot of pair correlation as a function of \( \phi(t)/\phi_0 \) and distance \( r \), for the 12 site ring with \( U = 2.0 \) and filling factors (a) \( f = 4/12 \) and (b) \( f = 6/12 \) with electric field strengths \( F = 0.0005 \) (top panel) and 0.5 (bottom panel). The color bar represents the numerical values of \( \langle P(r) \rangle \).

### Figure 8
Plot of time-averaged current, \( \langle J \rangle \) as a function of \( FL \) for different values of attractive interaction \( U \) with filling factors (a) \( f = 4/12 \) and (b) \( f = 6/12 \).
doping reduces the degeneracy and fades away the fractional periodicity. We observe that the applied field breaks the electron-pairs, namely the Cooper-pairs in these rings, driving the system from a superconducting to a metallic phase. The required strength of this applied field depends on the strength of the attractive interaction potential. Our study on the non-equilibrium behavior of the superconducting rings will drive further experiments to explore the rich phase diagram of the strongly correlated low-dimensional systems under external perturbations.

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