Optimizing the Cooper pair splitting efficiency in a Y-shaped junction

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(Dated: May 13, 2014)

This letter is devoted to the optimization of the Cooper pair splitting efficiency in a Y-shaped junction. The latter consists of two quantum dots, one superconducting and two normal leads. We tailor the bias in the two normal leads such that the Cooper pairs leaving the superconductor are split up resulting in entangled electrons, one on each quantum dot. We are able to achieve a splitting efficiency of more than 99% which is significantly better than the efficiencies obtained in experiments so far.

PACS numbers: 74.45.+c 03.67.Bg 73.63.-b 73.63.Kv

The entanglement of quantum particles has fascinated the scientific community since the proposition of the Einstein-Podolsky-Rosen Gedankenexperiment [1]. It is directly linked to the question of non-locality of quantum mechanics. A violation of Bell’s inequality would prove the latter [2]. Great progress has been achieved with entangled photons, but the final experiment ruling out all possible loopholes has not yet been accomplished [3]. To do similar experiments with electrons is much more difficult and remains an open challenge. In recent years, a number of ingenious experiments to create entangled electrons have been performed [4–6], going along with several theoretical developments [7–11]. The basic idea is to use a superconductor as a source of entangled electrons. In the BCS ground state, electrons form Cooper pairs due to the attractive interaction caused by phonons. These pairs consist of two electrons with opposite spin and momentum. The idea is to split the Cooper pairs by making them leave the superconducting lead, forcing one electron to move to a quantum dot on the left and the other to a quantum dot on the right (see sketch in Fig. 1). From these two quantum dots, the electrons are transported further into two metallic (normal-conducting) leads, L and R, where they get spatially separated. Since the splitting process does not affect the spin, the electrons are entangled because they stay in a spin-singlet state while separating. However, this process competes with the case of both electrons moving into the same lead. The latter can be suppressed by a large charging energy of the quantum dots caused by the Coulomb interaction. This make double occupancies less likely. The splitting further benefits from a weak coupling of the quantum dots to the leads compared to the superconducting gap [4]. Splitting efficiencies up to 90% have been realized in recent experiments [6] being significantly higher than previous results. Despite this progress, the experimental proof of the violation of Bell’s inequality is still pending.

In this letter, we propose a way to achieve splitting efficiencies of 99% and more, which we hope will help the eventual experimental demonstration of the violation of Bell’s inequality. The traditional approach to achieve high splitting rates relies on a large Coulomb repulsion on the quantum dots. The approach proposed in this letter is different: Our strategy is to use optimal control theory to tailor the bias in the normal leads in such a way that the splitting probability is maximized.

In order to describe transport processes through the Y-shaped junction sketched in Fig. 1 we consider the following model Hamiltonian:

\[
\hat{H}(t) = \sum_{\alpha \in \{L, R, S\}} \hat{H}_\alpha + \sum_{\alpha \in \{L, R\}} \hat{H}_{T, \alpha}(t),
\]

\[
\hat{H}_\alpha = \sum_{k=0}^{\infty} \sum_{\sigma \in \{\uparrow, \downarrow\}} \left( t_{\alpha} \hat{c}_{\alpha k\sigma}^\dagger \hat{c}_{\alpha (k+1)\sigma} + \text{h.c.} \right)
\]

\[
+ \sum_{k=0}^{\infty} \left( \Delta_{\alpha} \hat{c}_{\alpha k\uparrow}^\dagger \hat{c}_{\alpha k\downarrow} + \text{h.c.} \right) \text{ for } \alpha \in \{S, L, R\},
\]

\[
\hat{H}_{T, S} = \sum_{\alpha \in \{L, R\}} \sum_{\sigma \in \{\uparrow, \downarrow\}} \left( t_{S, QD_\alpha} \hat{c}_{S0\sigma}^\dagger \hat{d}_{QD_\alpha \sigma} + \text{h.c.} \right)
\]
\[ \hat{H}_{T,\sigma}(t) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \left( t_{\alpha, \text{QD}, \alpha} e^{i\gamma_{\alpha, \text{QD}, \alpha}(t)} \hat{c}^{\dagger}_{\alpha \sigma} \hat{d}_{\text{QD}, \sigma} + \text{h.c.} \right) \]

for \( \alpha \in \{L, R\} \) \hspace{1cm} (4)

with the Peierls’ phases \( \gamma_{\alpha, \text{QD}, \alpha}(t) = \int_0^t dt' U_{\alpha}(t') \) and the biases \( U_{\alpha}(t), \alpha \in \{L, R\} \). The operator \( \hat{c}^{\dagger}_{\alpha \sigma} \) (\( \hat{c}_{\alpha \sigma} \)) creates (annihilates) an electron at site \( k \in \mathbb{N} \) in the lead \( \alpha \in \{S, L, R\} \) with spin \( \sigma \in \{\uparrow, \downarrow\} \). The operator \( \hat{d}_{\text{QD}, \sigma}^{\dagger} \) (\( \hat{d}_{\text{QD}, \sigma} \)) represents the creation (annihilation) of an electron on the quantum dot \( \alpha \in \{L, R\} \).

All parameters in equations (1) - (3) are chosen real and positive. We shall work at temperature \( T = 0 \) and assume the wide band limit \( t_{\alpha, \text{QD}, \alpha} \ll t_{\alpha} \). In this limit, the results only depend on the ratios \( \Gamma_{\alpha, \text{QD}, \alpha} = 2t_{\alpha, \text{QD}, \alpha}^2 / t_{\alpha} \) but not on the hopping elements individually.

The pairing potentials can be written as \( \Delta_\alpha = \xi_\alpha \tilde{\Delta} \) which allows a dimensionless representation of the problem by measuring times in units of \( \tilde{\Delta}^{-1} \) and energies in units of \( \tilde{\Delta} \). We set \( \xi_S = 1 \) for the superconducting lead \( S \) and \( \xi_L = \xi_R = 0 \) for the other two. Due to the presence of superconductivity, we have to solve the time-dependent Bogoliubov-de Gennes equation, which is a Schrödinger-like equation in electron-hole space.

For the single particle wave functions \( \psi_q(k, t) = [u_q(k, t), v_q(k, t)]^\dagger \) it reads as follows:

\[
\frac{i}{\hbar} \frac{d}{dt} \begin{pmatrix} u_q(k, t) \\ v_q(k, t) \end{pmatrix} = \begin{pmatrix} H_{kl}(t) & \Delta_{kl} \\ \Delta_{kl}^\dagger & -H_{kl}(t) \end{pmatrix} \begin{pmatrix} u_q(l, t) \\ v_q(l, t) \end{pmatrix}, \hspace{1cm} (5)
\]

\[
H_{kl}(t) = \begin{pmatrix} h_{kl}(t) & \Delta_{kl} \\ \Delta_{kl}^\dagger & -h_{kl}(t) \end{pmatrix}. \hspace{1cm} (6)
\]

The algorithm for the time propagation of the single particle wave functions \( \psi_q(k, t) \) as well as the initial state calculation is explained in the work of Stefanucci et. al. [12], which extends the method of Kurth et. al. [13] to superconducting leads. The initial state is chosen to be the ground state of the system.

In the following, we demonstrate how to optimize the Cooper pair splitting efficiency in the above model of a two-quantum dot Y-junction. The goal is to operate the device as a Cooper pair splitter that creates entangled electrons on the two quantum dots. The splitting of a Cooper pair can be understood as a crossed Andreev reflection. An incoming electron in one of the normal leads gets reflected into the other lead as a hole. This creates a Cooper pair in the superconductor. The process is sketched in Fig. 2 (top left). Similarly, the opposition process removes a Cooper pair from the superconductor. Besides, there are three other possible reflection processes: (a) normal reflection, (b) Andreev reflection, and (c) elastic cotunneling. The latter corresponds to a reflection of the incoming electron to the opposite lead. These three processes together with the crossed Andreev reflection are all sketched in Fig. 2.

![FIG. 2. Overview of the four possible reflection processes. Black arrows indicate electrons, white arrows represent holes. The gray block is the superconducting lead S of Fig. 1. Top left: Sketch of a crossed Andreev reflection. The incoming spin up electron in the left lead gets reflected as a spin down hole to the right lead. Simultaneously, a Cooper pair is created in the superconducting lead. The opposite process, which removes a Cooper pair from the superconductor, is also possible. Bottom left: The reflected hole stays in the left lead. This corresponds to the normal Andreev reflection. Top right: Sketch of an elastic cotunneling process. Now, the incoming electron gets reflected into the right lead. Bottom right: Alternatively, the electron can also be reflected into the left lead corresponding to normal reflection.](image)

The central ingredient for the optimization process is the proper definition of a suitable objective function which is then to be maximized. It has to quantify the Cooper pair splitting efficiency. To this end, we first define the so-called pairing density or anomalous density as

\[
P_{\text{QD}, \text{QD}}(t) = \langle \hat{d}_{\text{QD}, \alpha, H}(t) \hat{d}_{\text{QD}, \beta, H}(t) \rangle. \hspace{1cm} (7)
\]

We use its absolute value squared \( |P_{\text{QD}, \text{QD}}(t)|^2 \) as a measure for the Cooper pair density with one electron at \( \text{QD}_\alpha \) and the other at \( \text{QD}_\beta \). We propose to maximize the following objective function:

\[
\frac{1}{t_1 - t_0} \int_{t_0}^{t_1} dt \frac{|P_{\text{QD}, \text{QD}}(t)|^2 + |P_{\text{QD}, \text{QD}}(t)|^2 + |P_{\text{QD}, \text{QD}}(t)|^2 + |P_{\text{QD}, \text{QD}}(t)|^2}{|P_{\text{QD}, \text{QD}}(t)|^2 + |P_{\text{QD}, \text{QD}}(t)|^2 + |P_{\text{QD}, \text{QD}}(t)|^2 + |P_{\text{QD}, \text{QD}}(t)|^2}. \hspace{1cm} (8)
\]
The fraction represents the Cooper pair splitting efficiency at time t, which is expressed as the amount of Cooper pairs being split up divided by the total amount of Cooper pairs on the quantum dots. We calculate its average over the time span from \(t_0\) to \(t_1\). The pairing densities \( \rho_{QD,\alpha QD,\beta}(t) \) are obtained from the single-particle wave functions \( \psi_q(t) \), i.e., the solutions of the time-dependent Bogoliubov-de Gennes equation (3).

We want to tailor the time-dependent bias such that the time averaged Cooper pair splitting efficiency, i.e. the objective function (3), is maximized. The numerical set-up to do this is by representing \( U_{\alpha}(t) \) by cubic splines with \( N+1 \) equidistant nodes at \( \tau_k = \frac{k}{N} T, k \in \{0, \ldots, N\} \).

The problem can be solved using standard derivative-free algorithms for non-linear optimization problems. This approach has already been used in several other works [14–17]. We use the algorithm BOBYQA [18] provided by the library NLopt [19]. It outperforms all other tested optimization algorithms.

To achieve high splitting efficiencies it is essential that the junction is asymmetric, i.e. the couplings to the left and to the right quantum dot must not be equal. This is necessary since we observe an upper bound of 50% for the Cooper pair splitting efficiency in symmetric junctions, which is already achieved in the ground state by the usual Cooper pair tunneling leading to the proximity effect. Hence any optimization starting in the ground state will not improve the results. We therefore choose an asymmetric coupling of the quantum dots to the normal leads.

The results of such an optimization are depicted in Fig. 3. The bias is tailored such that the Cooper pair splitting efficiency is maximized. It suppresses the non-splitting processes. The efficiency is optimized in the time interval from \(t_0 = 10\) to \(t_1 = 40\). This interval is indicated by the underlying thick gray line in the plot of the efficiency (middle). In this interval, we achieve an average efficiency of more than 99%. The values of \( |\rho_{QD_L,\alpha QD_R}(t)|^2 \) and \( |\rho_{QD_R,\alpha QD_L}(t)|^2 \) are on top of each other. This result demonstrates that the Coulomb interaction at the quantum dots is not necessary in order to obtain high efficiencies. One can also succeed with optimized biases.

To summarize, we have demonstrated how to optimize the Cooper pair splitting efficiency in a Y-shaped junction by suitably tailoring the bias. In this way, we are able to achieve splitting efficiencies of 99% and more, which is significantly higher than present experiments. This efficiency may help to finally demonstrate a violation of Bell’s inequality with electrons.
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