Can Negative Capacitance Induce Superconductivity?

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(Dated: 19 January 2022)

Superconductivity was originally observed in 3D metals caused by an effective attraction between electrons mediated by the electron-phonon interaction. Since then there has been a lot of work on 2D conductors including the possibility of alternative mechanisms that can lead to an effective attractive interaction. Inspired by the experimental demonstration of both steady-state and transient negative capacitance in a variety of structures, this paper investigates the possibility of superconductivity in a two-dimensional conductor embedded in a negative permittivity medium whose role is to turn the normally repulsive Coulomb interaction into an attractive one. A weak coupling BCS theory is used to identify the key parameters that have to be optimized to observe a superconducting transition, especially the need for a small effective negative permittivity, which could be obtained by balancing a negative permittivity medium with a positive permittivity one.

I. INTRODUCTION

Superconductivity is an intriguing phenomenon that is believed to arise in a wide variety of many-fermion systems due to two-body attractive interactions which introduce a very special kind of correlation among the one-fermion states. This state is commonly described by the Bardeen-Cooper-Schrieffer (BCS) theory [BCS 1957, PWA 1958, MLC 1964, PBA 1982] which was originally advanced to describe the superconducting state in 3D metals caused by an effective attraction between electrons mediated by the electron-phonon interaction. Since then there has been a lot of work on 2D superconductors which introduce many subtle issues summarized in a recent review [SAI 2021]. The recent discovery of superconductivity in twisted bilayer graphene has led to increased interest in 2D superconductivity including the possibility of alternative mechanisms that can lead to an effective attractive interaction, see for example, [BLG 2018, CEA 2021].

An enhancement in the superconducting transition temperature by \( \sim 0.15K \) was observed experimentally in a random mixture of superconducting (tin) and ferroelectric (barium titanate) nanoparticles and the observation was analyzed in terms of epsilon near zero (ENZ) conditions (MET 2014, 2015). This paper is based on somewhat similar physics but is inspired by the recent demonstration of negative capacitance (NC) in a variety of ferroelectric materials and structures, which we believe can be exploited to induce superconductivity at relatively high temperatures. The NC state of a ferroelectric is thermodynamically unstable, and two possible approaches have been identified for accessing it as summarized in [MH 2021]. The first is to stabilize it by placing it in series with a normal insulator with a positive permittivity as originally proposed in [SSD 2008]. In this case, stability requires the overall capacitance to be positive, though individual spatial domains have been shown to be in an NC state [SSS 2019]. The second is to switch the ferroelectric from one stable state to another such that it is in a transient NC state for times \( \sim \) tens of microseconds [SSA 2015]. Either the stabilized NC or the transient NC could possibly be used to demonstrate the phenomenon explored in this paper, but the latter seems more accessible experimentally, especially since transient NC is now a well-established phenomenon that has been measured by many groups using the experimental technique demonstrated in [SSA 2015].

With this in mind, we consider the idealized structure shown in Fig.1a with a 2D conductor sandwiched between two media, one having a negative permittivity \( -\epsilon_1 \), and one with positive permittivity \( +\epsilon_2 \). A possible experimental structure is sketched in Fig.1b with a conducting layer on a ferroelectric insulator (see for example, FEG 2021) or a ferroelectric semiconductor recently demonstrated in [PY 2019]. The ferroelectric is assumed to be in a negative capacitance state perhaps temporarily while it is switching polarizations. In this paper the permittivities are assumed to be isotropic. In practice, the orientations of the ferroelectric materials should be carefully designed to maximize the effective attraction. We
also note that the concept of negative capacitance goes beyond ferroelectric materials and could be engineered in magnetoelectric materials [KYC 2018] and other two-state systems separated by an energy barrier as noted in [SSA 2015].

The standard Coulomb interaction energy between two electrons in a 2D conductor embedded in a medium with a dielectric constant \( \epsilon_0 \) can be written as

\[
V(q) = \frac{e^2}{C(q)}
\]  

(1a)

where \( C(q) = 2\epsilon_0 A(q + \lambda) \), \( A \) being the area of the conductor, \( q \) the wavenumber and \( \lambda \) the inverse 2D screening length. For the structure shown in Fig.1, we modify this expression to account for the two different dielectrics and their finite thicknesses:

\[
C(q) = A \left( \frac{-\epsilon_1 q}{\tanh(qd_1)} + \frac{\epsilon_2 q}{\tanh(qd_2)} + \frac{2\pi m q^2 F}{\pi \hbar^2}q \right)
\]  

(1b)

where \( m \) is the effective mass of the electrons and \( v \) the number of valleys in the 2D conductor. The factor \( F \) equals one for small wavenumbers, but decreases significantly for wavenumbers \( \sim 2k_f \), \( k_f \) being the Fermi wavenumber related to the electron density \( n_s \) by \( k_f = \sqrt{2\pi n_s/v} \) [SCR 2015].

It is clear from Eq.1b that with proper design the capacitance \( C(q) \) can be negative. The interaction then becomes an attractive one, potentially capable of inducing a transition to a superconductor-like state in the 2D conductor. We show that the corresponding transition temperature \( T_c \) is given by a BCS-like expression

\[
\Delta(T \to 0) \approx \frac{\min(h\omega_0, E_f)}{\sinh(\alpha)}
\]  

(2a)

where \( \Delta(T) \) is the pair potential, \( \omega_0 \) is the high frequency cut-off for the dielectric response, \( E_f \) is the Fermi energy of the 2D conductor and \( \alpha \) is the dimensionless coupling constant given by

\[
\alpha = \frac{e^2 m \langle \ell_s \rangle}{4\pi \epsilon_0 \hbar^2}
\]  

(2b)

where \( \langle \ell_s \rangle \) is the average value of an effective length defined in terms of the inverse negative capacitance:

\[
\ell_s(k, k') = \frac{\epsilon_0 A}{2\pi} \int_0^{2\pi} \frac{d\theta}{q = \sqrt{\epsilon_2 + k^2 + 2k k' \cos \theta}}
\]  

(2c)

\( k, k' \) being wavevectors for states with energies within \( h\omega_0 \) of the Fermi energy \( E_f \). The coupling constant \( \alpha \) in Eq.2b plays the role of "\( N(0)/V \)" in BCS theory. Indeed it is equal to the product of the two-dimensional density of states \( m/2\pi \hbar^2 \) and the approximate attractive interaction energy \( e^2 \langle \ell_s \rangle/2\epsilon_0 \).

Multi-valley semiconductors introduce additional contributions from terms where \( k, k' \) belong to different valleys, but in the following discussion we will assume a single valley \( (v = 1) \).

II. RESULTS

A key point that emerges from Eq.2a is that to observe the superconducting transition we need to design structures that maximize \( \alpha \) and hence \( \ell_s \), which in turn requires \( C(q) \) to have a small negative value at least over a significant range of \( \theta \). One way to achieve this is to choose \( \epsilon_1, \epsilon_2 \) such that for small \( q \) the quantity \( (v = 1) \)

\[
-\frac{C(q \to 0)}{A} \approx \frac{\epsilon_1}{d_1} - \frac{\epsilon_2}{d_2} - \frac{e^2 m}{\pi \hbar^2}
\]

has a small positive value. For example, if \( d_1 = d_2 = d \), we choose

\[
\epsilon_1 - \epsilon_2 \approx K \frac{e^2 m d}{\pi \hbar^2}
\]

(3a)

so that from Eqs.2b,2c

\[
\alpha \approx \frac{1}{8\pi} \int_0^{2\pi} \frac{d\theta}{K q d / \tanh(qd) - F}
\]

(3b)

\( K \) is a positive number a little larger than one, so that for small \( q \) the integrand, \( 1/(K - 1) \), is large.

![Fig. 2. Pair potential \( \Delta(T) \) calculated from Eq.6b using two values of the constant \( K \) (see Eq.3a) as indicated. Other parameters are described in the text. The numerical values of \( \Delta(T \to 0) \) agree well with Eq.2a using \( \alpha \) from Eq.3b.](image)

As an example, we choose \( d_1 = d_2 = d = 4nm \) with \( m = 0.25m_0 \) and electron density, \( n_s = 10^{16}/m^2 \). The net negative permittivity, \( \epsilon_1 - \epsilon_2 \approx 80\epsilon_0 \) as obtained from Eq.3a and the factor \( F \) is set equal to its small wavenumber value of one. We use \( \omega_0 = 2 \text{THz} \), comparable to the lowest atomic vibration frequency in \( HfO_2 \) based systems [HFO 2012]. Fig.2 shows the pair potential \( \Delta(T) \) calculated numerically from Eq.6b for two values of \( K = 1.1 \) and \( 1.01 \), corresponding to coupling constants \( \alpha \) of \( \sim 0.66 \) and \( \sim 2.13 \) respectively.
III. METHODS

A. Model

Consider a two-dimensional conductor described by a parabolic band $\epsilon_k = \hbar^2 k^2 / 2m$ so that the non-interacting system is described by

$$ H_0 - \mu N = \sum_k (\epsilon_k - \mu) c_k^\dagger c_k $$  (4a)

Here $\mu$ is the equilibrium chemical potential equal to the Fermi energy $E_f = \hbar^2 k_f^2 / 2m$. The electron-electron interaction is described by

$$ H_{\text{int}} = \sum_{k,k',\beta,s',s} V(q) c_{k',s'}^\dagger c_{\beta-k',s'} c_{\beta-k,s} c_{k,s} $$  (4b)

where $s,s'$ are the spin indices, $q = |\mathbf{k}-\mathbf{k}'|$ and $V(q)$ is the interaction energy from Eqs.1a,1b.

B. Gap equation

It is well-established that any attractive interaction like Eq.3b can lead to a superconducting phase having a non-zero pair potential $\Delta_k \equiv \langle c_{-k,\downarrow} c_{+k,\uparrow} \rangle$ which can be calculated by solving the BCS gap equation self-consistently:

$$ \Delta_k = \frac{1}{2} \sum_{k'} -V(|\mathbf{k}-\mathbf{k}'|) \frac{\Delta_{k'}}{E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \times \vartheta (\hbar \omega_0 - |\epsilon_{k'} - \epsilon_k|) $$  (5a)

where $E_{k'} = \sqrt{(\epsilon_{k'} - \mu)^2 + \Delta_{k'}^2}$.

Here we have added the last term in with the step function $\vartheta$ in Eq.6a to account approximately for the high frequency response of the dielectric response, similar to the Debye frequency used for the electron-phonon interaction in BCS theory. A full Green’s function formalism could be used for a more quantitative analysis.

Defining an effective thickness

$$ \ell_s(k,k') \equiv \frac{\epsilon_0 A}{2\pi} \int_0^{2\pi} \frac{d\theta}{C(q)} \bigg|_{q=\sqrt{k^2+k'^2-2kk\cos\theta}} $$  (6a)

we can rewrite Eq.4a by substituting from Eqs.1a,1b and converting the summation into an integral:

$$ \Delta_k = \frac{1}{2} \frac{A}{4\pi^2} \int_0^{2\pi} \frac{d\kappa'}{C(q)} \Delta_{k'} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \times \frac{2\pi e^2}{\epsilon_0 A} \ell_s(k,k') \vartheta (\hbar \omega_0 - |\epsilon_{k'} - \epsilon_k|) $$  (6b)

C. Approximate solution

Replacing $\ell_s(k,k')$ with its average value, we can write Eq.5a

$$ \Delta_k \approx \frac{\epsilon^2 m}{4\pi \epsilon_0 \hbar^2} \int_{\pi - \delta}^{\pi + \delta} \frac{d\epsilon_{k'}}{\epsilon_{k'}} \Delta_{k'} \tanh \left( \frac{E_{k'}}{2k_B T} \right) $$  (7)

where $\delta = \min(|\hbar \omega_0, E_f|)$. As $T \to 0$ assuming a constant $\Delta$ in the energy range between $\mu - \delta$ and $\mu + \delta$

$$ \Delta \approx \frac{\alpha}{\sqrt{(\epsilon_{k'} - \mu)^2 + \Delta^2}} \int_{\mu - \delta}^{\mu + \delta} \frac{\Delta}{\sqrt{y^2 + \Delta^2}} \left( \sinh^{-1}(\delta/\Delta) \right) $$

This leads us to the approximate result cited earlier in Eq.2a.

D. Multi-valley conductors

Finally we note that the conduction band in many semiconductors have a number of equivalent valleys, $v$ such that $n_s = v \times k_f^2 / 2$. The gap equation is modified from Eq.5a to include a sum over the equivalent valleys. However, the intervalley terms involve large values of $\epsilon$ which require more careful discussion.

IV. CONCLUDING REMARKS

In summary, this paper draws attention to the possibility of engineering heterostructures that could provide a new route to superconductivity, based on the recent demonstration of negative capacitance, steady-state or transient. A simple treatment is presented showing that the transition temperature can be estimated from a BCS-like expression (see Eq.2a) with the coupling constant given by Eq.2b which plays the role of $N(0)V$ in conventional superconductivity. This expression is used to identify the key parameters that need to be optimized to observe a superconducting transition, especially the need for a small negative permittivity, which could be obtained by balancing a negative permittivity medium with a positive permittivity one. Negative capacitance can arise in other material systems as well and it may be possible to engineer heterostructures with coupling constants in excess of one, leading to higher transition temperatures.
ACKNOWLEDGMENTS

The author is grateful to Prof. Sayeef Salahuddin for alerting him to transient NC and for helpful discussions regarding negative permittivity in ferroelectrics. He is also indebted to Prof. Pramey Upadhyaya for his help with screening in 2D conductors. It is a pleasure to thank Prof. Bhaskaran Muralidharan, Kerem Camsari and Zubin Jacob for their feedback on the manuscript. This work was supported by the Purdue Research Foundation.

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