Excitonic condensation in spatially separated one-dimensional systems

D. S. L. Abergel
Nordita, KTH Royal Institute of Technology and Stockholm University,
Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden.

We show theoretically that excitonic condensation can take place in a variety of one-dimensional systems. We describe the mean-field Bardeen-Cooper-Schrieffer theory which is applicable to a wide class of one-dimensional setups, and then focus on the core-shell nanowire for which we give estimates of the size of the excitonic gap for a specific InAs/GaSb wire, and as a function of all the experimentally relevant parameters. We find that even when static screening of the inter-layer interaction is taken into account (which tends to under-estimate the strength of the Coulomb interaction), that a superfluid gap of the order of Kelvin is achievable, demonstrating that the one-dimensional excitonic condensation is substantially more robust than the frequently-studied two-dimensional one.

Excitonic condensation is the formation of a macroscopic condensed state from paired electrons and holes. The quasiparticles which comprise this boson may come either from optically pumped (and hence transient) states, or from spatially separated long-lived populations such as an electron-hole bilayer. The latter has a long history of consideration in two dimensions (2D), where firstly semiconductor heterostructures [1], and more latterly, double graphene layers [2, 3] were proposed as systems where this phenomenon could be observed. However, the only clear experimental evidence for such a state has been seen in a strong magnetic field [4], and despite much effort, the excitonic condensate has not been observed in zero field [5–7].

Such excitonic condensation cannot formally exist in one dimension (1D) in the true sense of having long-range order, but exciton correlations may exist at finite length scales and are characterised by a power law decay. We propose that this partial condensation may be supported in various condensed matter systems including stacked graphene nanoribbons [8], in nanowires or carbon nanotubes arranged side-by-side, or in a core-shell nanowire (CSN). These setups are illustrated schematically in Fig. 1. The CSN is a particularly interesting case since it has recently been demonstrated that certain combinations of core and shell materials allow for simultaneous populations of holes in the core region and electrons in the shell region, minimal coupling between the two, and ambipolar transport characteristics [9]. However, in all three candidate systems, the important experimental prerequisites are that the electron and hole populations are simultaneously produced and independently contacted. Independent contacting of the two layers is essential to allow experimental detection of the formation of the condensate, either via Coulomb drag measurements [10], or via a change in the tunneling current between the two layers [4]. In the case of stacked graphene, this has been demonstrated many times in 2D since the two layers can be gated from opposite sides [11] and contacting the two layers is also straightforward. Also, the growth process of CSNs will allow this since it is possible to grow the shell around only some region of the core and hence leave both materials exposed for independent contacting.

Previously, excitonic condensation has been considered in 1D in the context of the high density limit of optical excitations [11]; BCS theory was applied to cold fermionic gases generally using a short-range interaction [12–16], in carbon nanotubes [17], and in a non-equilibrium context [18]; but, to the best of our knowledge, only once for spatially separated systems using the language of bosonization [19].

In this article, we present the 1D BCS theory that is applicable for all spatially separated electron and hole systems. We shall then give numerical results which illustrate the behavior of such a system in the ideal case with and without screening in the inter-layer interaction. Finally, we discuss some specific practical details of CSN systems, and how excitonic condensation would differ in the other possible setups.

We begin by writing the Hamiltonian in the notation $H = H_{SP} + V$ where $H_{SP}$ contains the single particle terms and $V$ is the inter-layer interaction. Throughout, we assume that intra-layer interactions only have the direct effect of renormalizing the single particle band parameters but will also play an indirect role via the screen-
ing of the inter-layer interaction. We assume that both the electron and hole regions contain one non-degenerate band and allow for independent chemical potentials in each region \[20\]. The annihilation operator for an electron in one of these bands is denoted \( \epsilon_{ik} \) where \( b = 1, 2 \) denotes the band, and \( k \) is the momentum. Since we enforce one band to be electron-like and the other to be hole-like we introduce the following notation: \( \epsilon_{ik} = c_{ik} \) is the annihilation of an electron in layer 1, and \( b_{-k} = c_{ik}^\dagger \) is the annihilation of a hole in layer 2. The single-particle part of the Hamiltonian is

\[
H_{\text{SP}} = \sum_k \xi_{ik} a_k^\dagger a_k + \sum_k \xi_{2k} b_{-k}^\dagger b_{-k}.
\]

with \( \xi_{ik} = \epsilon_{ik} - \mu_1 \) and \( \xi_{2k} = \epsilon_{2k} - \mu_2 \). The inter-layer interaction between the electrons and holes exists within the standard mean-field BCS theory and the resulting interaction Hamiltonian is:

\[
V = \sum_k \Delta_k a_k^\dagger b_{-k}^\dagger + \text{h.c}
\]

where the superfluid gap \( \Delta_k \) is defined as the self-consistent solution of the equation

\[
\Delta_k = \frac{1}{\pi} \int \frac{dk'}{2\pi} V_{-\h}(k' - k) \frac{\Delta_{k'}}{\sqrt{\xi_1 - \xi_2}^2 + 4\Delta_{k'}^2}.
\]

The quantity \( V_{-\h}(q) \) is the Fourier transform of the inter-layer interaction. In the unscreened case, it is

\[
V_{\text{inter}}(q) = -2e^2/\kappa K_0(|k|d).
\]

where \( K_0(z) \) is the modified Bessel function of the second kind and \( \kappa \) includes the relative permittivity of the surrounding medium. The minus sign appears because each 1D system contains carriers of opposite charge so that their Coulomb interaction is attractive. This Hamiltonian is diagonalized using a Bogoliubov transformation which yields two excitonic bands with dispersion

\[
E_{\pm,k} = \pm \frac{\xi_{ik} + \xi_{2k}}{2} + \frac{1}{2} \sqrt{(\xi_{ik} - \xi_{2k})^2 + 4\Delta_k^2}.
\]

This indicates that, for finite \( \Delta_k \), a gap opens in the single particle spectrum near the points where the two bands cross, and the magnitude of this gap is exactly \( \Delta_k \) evaluated at the wave vector of the crossing point.

We can arrive at a crude analytical expression for the size of the excitonic gap for the unscreened inter-layer interaction by approximating the inter-layer interaction as \( V_{\text{inter}} = -2e^2/\pi \delta(q) \). Substituting this into Eq. (1) we obtain the maximum value of the gap function as \( \Delta_{\text{max}} \approx e^2/(4\pi^2 \kappa d) \). This will underestimate the strength of the pairing interaction, since it excludes interaction at finite \( k - k' \) so that the actual unscreened gap will exceed this estimate.

There is an extensive literature covering the screening of the inter-layer interaction in the 2D double layer graphene setup \[21\,24\]. The calculation of screening cannot be done exactly, and therefore some approximation has to be made. In the static limit of the random phase approximation, this is done by replacing the constant dielectric function \( \kappa \rightarrow \kappa \bar{\kappa} \) where, for a two component system \[25\],

\[
\bar{\kappa} = 1 - V_{\text{intra}}(q)[\Pi_{11}(q,0) + \Pi_{22}(q,0)] + [V_{\text{intra}}(q)]^2[\Pi_{11}(q,0)\Pi_{22}(q,0)]
\]

where \( V_{\text{intra}}(q) \) and \( V_{\text{intra}}(q) \) are, respectively, interaction between carriers in opposite layers or the same layer, and \( \Pi_{ii}(q, \omega) \) is the non-interacting frequency-dependent polarization function in layer \( i \). The inter-layer interaction is given in Eq. (2), but the Fourier transform of the intra-layer interaction is divergent due to the infinite contribution at \( x = 0 \). Therefore, we make the assumption that this divergence is cut off by the radial size of the wave function and

\[
V_{\text{intra}}(q) = \frac{2e^2}{\kappa} K_0(|k|d).
\]

We discuss physical justifications for the choice of cutoff below. The positive sign in front of this interaction occurs because the charges within a layer are the same so that their Coulomb interaction is repulsive. For a spinless 1D system, the intra-layer polarization function is

\[
\Pi_{ii}(q, \omega) = \frac{1}{2\pi} \int_{-\infty}^\infty n_F(k) - n_F(k + q) d\omega
\]

where \( n_F(k) \) is the occupation of state \( k \) and \( \eta \) is a positive infinitesimal. This can be evaluated numerically for a given band structure. In this work, we focus on the statically screened interaction. This approximation is known to over-estimate the strength of the screening, and therefore gives a lower bound on the value of the mean-field gap \[20\]. Conversely, the unscreened interaction is clearly an over-estimation of the interaction strength, and therefore represents an upper bound on the stability of the condensate. We shall demonstrate below that, for physically reasonable parameters, both these models for screening produce an estimate for the zero temperature excitonic gap which are at most one order of magnitude different from each other.

The theory outlined above is completely general for all spatially separated 1D electron-hole systems. However, to give a concrete example and experimentally relevant predictions, we make our theory specific to the CSN. Here, it is reasonable to approximate the low energy band structure in a quadratic form \[27\,28\] parameterized by a band offset \( E^\text{ext} \) and an effective mass \( m^* \) such that

\[
\epsilon_{ik} = E^\text{ext}_i + \frac{p^2 k^2}{2m^*_i},
\]

where \( i \) denotes the electron or hole part of the wire. One combination of materials of particular interest is a CSN with a core (hole) region of GaSb and a shell
FIG. 2. Predicted $\Delta_{\text{max}}$ as a function of layer separation for an InAs/GaSb core-shell nanowire as a function of (a) effective separation $d$ and (b) the chemical potential $\mu$. Other parameters are specified in the text.

(electron) region of InAs $\text{[9]}$. Using parameters from Ref. 27 we take band extrema of $E_{\text{InAs}}^{\text{ext}} = -0.2eV$ and $E_{\text{GaSb}}^{\text{ext}} = -0.05eV$, and effective masses of $m_{\text{InAs}} = 0.02$ and $m_{\text{GaSb}}^* = -0.07$. This pair of materials fulfills the general requirements for the condensate to exist: that the effective masses have opposite sign, and that the bands overlap. We assume a dielectric constant of $\varepsilon_r = 12$ in both materials (where $\kappa = 4\pi\varepsilon_0\varepsilon_r$ in SI units). The pairing happens most strongly when the chemical potential $\mu$ is placed at the point where the two bands cross, given by $\mu_e = (m_1^e E_{\text{InAs}}^{\text{ext}} - m_2^e E_{\text{GaSb}}^{\text{ext}})/(m_1^e - m_2^e)$. Below, we examine the stability of the condensate against changing $\mu$, but for now we keep $\mu = \mu_c$.

Figure 2(a) shows the predicted maximum of the gap function $\Delta_{\text{max}}$ for a InAs/GaSb CSN for both the unscreened and statically screened interaction. The high value of the dielectric constant means that the screening is relatively weak and, for larger values of $d$, the two interactions give gap functions of the same order of magnitude. Even at smaller $d$, the difference is only one order of magnitude, which is far smaller than in the 2D graphene case $\text{[25]}$. However, the estimated gap size is of the order of a few Kelvin at best. Also, in Fig. 2(a) we show two different values of the small distance cutoff in the intra-layer interaction. The value of 1nm corresponds to choosing the cutoff to coincide with the order of magnitude of the radial spread of the electronic wavefunction within the core or the shell layer, while the value of 0.1nm is the value taken to represent a cutoff of the order of the lattice constant. Both values give almost indistinguishable results for the gap size. This figure shows that core-shell nanowires have a substantial advantage over double layer graphene systems because the screening plays a much smaller role.

Figure 2(b) shows how $\Delta_{\text{max}}$ behaves as a function of the chemical potential. As $\mu$ moves away from $\mu_c$, the gap stays unchanged until a certain point where it collapses to zero immediately. This is caused by the minima of the excitonic bands $E_{\pm,k}$ becoming negative and allowing for gapless excitations at the Fermi energy which are energetically favorable to the condensate state. Assuming the gap is described $\Delta_{\text{max}}$, the value of the chemical potential for which this happens $\mu_{\text{crit}}$ is

$$\mu_{\text{crit}} = \mu_c \pm 2\Delta_{\text{max}} \sqrt{|m_1^e||m_2^e|}/|m_1^e - m_2^e|.$$  \hspace{1cm} (5)

This is true for both the unscreened and statically screened cases, and for the parameters appropriate to the InAs/GaSb wire, we find $\mu_{\text{crit}} = \mu_c \pm 0.83\Delta_{\text{max}}$. The coefficient of $\Delta_{\text{max}}$ in the second term is peaked when $m_1^e = -m_2^e$ indicating that the condensate is the most robust against shifts in the chemical potential in this case.

In principle, the choice of material for the core and shell regions could be made so as to optimize the strength of the condensate. Therefore, we analyze $\Delta_{\text{max}}$ as a function of the band parameters and dielectric constant. Figure 2(a) shows $\Delta_{\text{max}}$ for the unscreened interaction as a function of the overlap of the two bands such that $E_{\text{InAs}}^{\text{ext}} = -E_{\text{GaSb}}^{\text{ext}} = E_{\text{2D}}^{\text{ext}}$ for three different values of the effective masses defined such that $m^* = m_1^e = -m_2^e$. We fix all other parameters. This indicates that the pairing is strongest when $\mu_c$ is close to the band extrema. Figure 2(c) shows $\Delta_{\text{max}}$ as a function of the band masses. Here, we rearrange them such that $\tilde{m} = (|m_1^e| + |m_2^e|)/2$ and

FIG. 3. Role of band parameters in the size of the excitonic gap. (a) $\Delta_{\text{max}}$ as a function of the band overlap for the unscreened inter-layer interaction. We fix $d = 5nm$ and $\varepsilon_r = 4$. (b) $\Delta_{\text{max}}$ as a function of $\varepsilon_r$ for the unscreened and statically screened inter-layer interactions. We use $d = 5nm$ and band parameters suitable for an InAs/GaSb wire. (c) $\Delta_{\text{max}}$ as a function of $\tilde{m}$ and $d/\sqrt{\pi}\kappa$. Below, we examine the stability of the condensate against changing $\mu$, but for now we keep $\mu = \mu_c$.

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\( \delta m = |m^*_1| - |m^*_2| \) while fixing the criteria that \( m^*_1 > 0 \) and \( m^*_2 < 0 \). The unfilled region in the upper-left part of the plot denotes where these criteria cannot be fulfilled. Looking first along the \( \delta m = 0 \) axis, we see that \( \Delta_{\text{max}} \) increases with the band masses. This, taken together with the observations from Fig. 3(a) indicate that having flat bands (and hence a higher density of states) makes the condensate more robust. Allowing \( \delta m \) to be finite shows that imbalance in the two effective masses is detrimental to the condensate. Figure 3(b) shows that the dielectric constant of the medium is also a crucial parameter. We find that in the statically screened case, the suppression of pairing is exponential in \( \epsilon_r \), while for the unscreened interaction the suppression is slightly sub-exponential. Also, as expected from the consideration of the screening properties above, higher dielectric constant reduces the effectiveness of the screening and means that the unscreened and statically screened results become more similar to each other.

Since we focus on the CSN system where there is no spacer layer between the electron and hole regions, we have to take the possible direct tunelling of carriers between the two bands, and the resulting hybridization of the single particle bands into account. The hybridization of bands in the context of 2D excitonic condensation has been analyzed previously \([23, 24]\) where it was found that a small hybridization was beneficial to the formation of a gap at the Fermi energy.

The situation with graphene nanoribbons will be qualitatively similar to that discussed for CSNs. For armchair nanoribbons, the dispersion associated with the single particle bands will change to \( \epsilon_{ik} = \pm \sqrt{k_0^2 + k^2} \) where the sign reflects the conduction or valence band, and \( k_0 \) is the extremum of the lowest subband and is set by the ribbon geometry \([3]\). A chirality factor resulting from the sublattice structure of the underlying graphene also has to be added to Eq. 1 which will manifest simply as a small quantitative change in the gap size. Also, the chemical potential of the two layers may be set independently, but the most advantageous situation will occur when the Fermi points in the two layers are at the same wave vector. For graphene systems, it is well known that the crystal lattice structure is of remarkably high quality, and that the dominant form of disorder is charged impurities trapped in the environment of the flake. In 2D, the effect of the fluctuations in the local charge density resulting from these impurities has been shown to be highly detrimental to the stability of the condensate \([30, 51]\). This will be no different for stacked graphene nanoribbons and so the result in Eq. (5) will characterise the stability of the condensate against local fluctuations in the chemical potential.

Dynamic (finite frequency) screening effects will reduce the strength of the screening and increase the stability of the condensate, relative to the static screening. It has also been shown in 2D systems that taking into account the screening by the condensate itself may have a substantial positive effect on the condensate \([23, 32]\). However, this effect is most noticeable for small values of the dielectric constant (or, in the language of Ref. 23, large values of the coupling constant \( \alpha \propto 1/\epsilon_r \)) so is not of particular interest in the study of CSNs where \( \epsilon_r \approx 12 \).

In conclusion, we have demonstrated that excitonic condensation in 1D systems has a realistic chance of being observed in a variety of experimental systems. In particular, CSNs provide a likely platform for its observation, with an excitonic gap of the order of Kelvin for thin wires. We wish to thank Martin Liejne, Claes Thelander, Bahram Ganjipour, and Alexander Balatsky for helpful discussions. This work was supported by ERC DM-321031 and by Nordita.

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