

# Exciton condensate modulation in electron-hole bilayers: A real-space visualization

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We study the texture of the exciton condensate at low temperatures in an independently gated electron-hole bilayer system. A model Hamiltonian is solved in real space within a mean-field approximation. It is found that, with increased electron-hole density polarization, the system experiences phase transformations from the zero center-of-mass momentum superfluid state, through one- and two-dimensional exciton pair modulated states, into the normal state. At weak density polarization, the modulating state resembles the Larkin-Ovchinnikov state in superconductors in the presence of an exchange field in the weak-coupling BCS limit and becomes stripe-like in the strong-coupling BEC limit. In the one-dimensional modulated phase, the density of states exhibits low-energy intragap resonance quasiparticle states, which are localized in the nodal region.

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## I. INTRODUCTION

The Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state<sup>1,2</sup> represents a class of unconventional superconducting states, where the superconducting order parameter modulates in *real space*. It is *dual* to the other more familiar class of unconventional superconducting states, in which the superconducting order parameter modulates (or even changes sign) in *momentum space*. In the FFLO state, the Cooper pairs form between two electrons with  $(\mathbf{k}+\mathbf{q}/2, \uparrow)$  and  $(-\mathbf{k}+\mathbf{q}/2, \downarrow)$  of momentum and spin configuration. The center-of-mass momentum  $\mathbf{q}$  is dependent on the extent to which the Fermi surface is Zeeman split by an exchange field. Although the FFLO state was predicted more than four decades ago, an undisputed verification of this state in superconductors remains a great experimental challenge. A major reason lies in the fact that, in most superconductors, the Pauli paramagnetic effect of the applied magnetic field is negligibly small compared with the orbital field breaking effect. Owing to recent advances in the discovery of new materials and new technology, there is a revival of interest in the FFLO-type modulated states in a wide range of systems. Among them, newly discovered heavy fermion superconductors,<sup>3-5</sup> low-dimensional organic superconductors,<sup>6-10</sup> and trapped cold Fermion atoms<sup>11-16</sup> are good candidates for the emergence of a superconducting FFLO state. In parallel, semiconductor bilayer systems<sup>17</sup> represent another promising context for the concept of FFLO-like states and the fundamental physics of the BCS-BEC crossover, in which there is condensation of electron and hole pairs.

In electron-hole bilayers, the density of the electrons and holes can be varied independently of each other. The effect of electron-hole density imbalance here resembles the exchange effect of an applied magnetic field in a superconductor. Such an effect on the BCS-BEC crossover in semiconductor electron-hole bilayers has recently been investigated at zero temperature by Pieri *et al.*,<sup>18</sup> where an instability toward the FFLO phase was identified. A more recent study,<sup>19</sup> by treating the FFLO phase and the Sarma phase<sup>20</sup> on an equal footing, indicated that the FFLO state can be stabilized by an order-parameter mixing effect. We note that, though collectively known as the FFLO state, the

form proposed by FF (Ref. 1) and that by LO (Ref. 2) are slightly different. In the FF form, the order parameter has a homogeneous magnitude but with a modulated complex phase factor, which is a single-wave-vector plane wave; while, in the LO form, the order parameter is real and spatially modulated. In Refs. 18 and 19, the authors solved the problem directly in momentum space, which limits consideration to the FF form. In this paper, we consider a simplified tight-binding model for an electron-hole bilayer and solve the BCS-type equation self-consistently in real space. It is found that the LO form is always stabilized. Of particular interest, we find a crossover from the LO state to an exciton stripe state as the pairing interaction is tuned from the BCS limit to the BEC limit. Our local-density-of-states calculations show the existence of intragap states, which are localized on the nodal lines, in the one-dimensional LO phase.

The paper is organized as follows. In Sec. II, a tight-binding model for the gated bilayer electron-hole system is introduced, and the Bogoliubov-de Gennes (BdG) formalism is presented. In Sec. III, we first show the texture of exciton pair order parameter in real space for varying strength of the polarization field and give a schematic phase diagram. The local electronic structure is also studied in the LO phase. In Sec. IV, we summarize our results.

## II. MODEL HAMILTONIAN AND THEORETICAL APPROACH

We start with a generic two-layer system, schematically shown in Fig. 1. The two layers are separated by an insulator such that the interlayer tunneling is negligible. The chemical potential in each layer can be tuned by gate voltages  $V_{g,+}$  and  $V_{g,-}$ . In the tight-binding model for a square lattice in each layer, the Hamiltonian can be written as

$$\mathcal{H} = \sum_{ij,\sigma} [-t_{ij,\sigma} - \mu_{\sigma}\delta_{ij}] c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} \sum_{ij,\sigma} g_{ij} n_{i,\sigma} n_{j,\bar{\sigma}}. \quad (1)$$

Here  $c_{i\sigma}^{\dagger}$  ( $c_{i\sigma}$ ) are the creation (annihilation) operators of an electron at site  $i$  in layer  $\sigma=1$  or  $2$ . The symbol  $\bar{\sigma}=2$  for  $\sigma=1$  and vice versa. The quantities  $t_{ij,\sigma}$  and  $\mu_{\sigma}=V_{g,\sigma}$  are the hopping integrals and chemical potentials in each individual

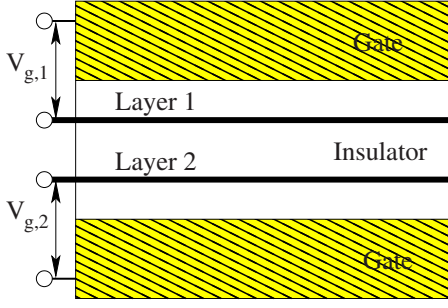


FIG. 1. (Color online) Schematic of a bilayer system. The carrier in each layer has electron or hole nature, which is determined by the individual band structure. The chemical potential in each layer is adjusted by the respective gate voltage.

layer, respectively. We introduce  $g_{ij}$  as the interlayer particle-particle coupling strength. In Hamiltonian (1), the particle-particle interaction within each individual layer is ignored, since they are expected to mainly renormalize each band. In our setting, explicit spin quantum numbers are omitted. As such, the index  $\sigma$  can be regarded as a pseudospin index, which we will use interchangeably,  $\sigma = +(-)$  or  $\uparrow(\downarrow)$ . In the mean-field approximation, the above Hamiltonian can be written as

$$\mathcal{H}_{\text{MF}} = \sum_{ij,\sigma} [-t_{ij,\sigma} - \mu_{\sigma}\delta_{ij}]c_{i\sigma}^{\dagger}c_{j\sigma} + \sum_{ij} [\Delta_{ij}c_{i1}^{\dagger}c_{j2} + \text{H.c.}] + \sum_{ij} |\Delta_{ij}|^2/g_{ij}, \quad (2)$$

where the order parameter is defined as  $\Delta_{ij} = g_{ij}\langle c_{i1}c_{j2}^{\dagger} \rangle$ . Through a canonical transformation, the above Hamiltonian can be diagonalized by solving the following BdG equation:

$$\sum_j \begin{pmatrix} h_{ij,1} & \Delta_{ij} \\ \Delta_{ji}^* & h_{ij,2} \end{pmatrix} \begin{pmatrix} u_j^n \\ v_j^n \end{pmatrix} = E_n \begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix}, \quad (3)$$

where the single-particle Hamiltonian and the pair potential are given by

$$h_{ij,\sigma} = -t_{ij,\sigma} - \mu_{\sigma}\delta_{ij}, \quad (4)$$

and

$$\Delta_{ij} = \frac{g_{ij}}{2} \sum_n u_i^n v_j^{n*} \tanh\left(\frac{E_n}{2k_B T}\right), \quad (5)$$

and  $(u_i^n, v_i^n)$  are the eigenvector corresponding to the eigenenergy  $E_n$ . The quasiparticle energy is measured with respect to the Fermi energy.

The above formalism is generic and applicable to both electron-electron or electron-hole bilayer systems, as determined by the band structure within each layer. Within the nearest-neighbor hopping approximation, the band dispersion for the uniform case can be written as

$$\xi_{k\sigma} = -2t_{\sigma}(\cos k_x + \cos k_y) - \mu_{\sigma}, \quad (6)$$

with  $t_1 > 0$  and  $t_2 > 0$  for the electron-electron bilayers, and  $t_1 > 0$  and  $t_2 < 0$  for the electron-hole bilayers. A schematic of normal-state band dispersion is shown in Fig. 2. Also the

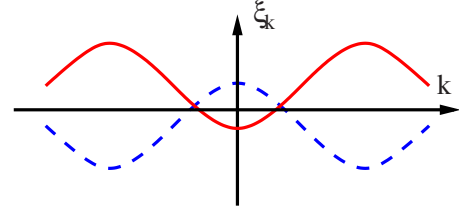


FIG. 2. (Color online) Schematic of the energy dispersion for electron (red-solid line) and hole (blue-dashed line) layers.

particle-particle interaction is long ranged when the screening effect is weak, as considered in usual coupled quantum wells, and short ranged when the screening effect is strong, which might be relevant when the metallic gate structures are present in the vicinity of quantum wells. For the purpose of the present discussion, we consider the electron-hole bilayer system, and consider a short-ranged Coulomb interaction with  $g_{ij} = g\delta_{ij}$  such that  $\Delta_{ij} = \Delta_i\delta_{ij}$ .

### III. NUMERICAL RESULTS AND DISCUSSIONS

We solve the above set of BdG equations self-consistently via exact diagonalization. Within the above mean-field treatment, the quasiparticle energy dispersion in the “quenched” uniform exciton condensate, that is,  $\Delta_i = \Delta_0$ , is of the form

$$E_{\pm}(\mathbf{k}) = \frac{\xi_{\mathbf{k},1} + \xi_{\mathbf{k},2}}{2} \pm \sqrt{\left(\frac{\xi_{\mathbf{k},1} - \xi_{\mathbf{k},2}}{2}\right)^2 + |\Delta_0|^2}. \quad (7)$$

From this energy dispersion form, one can see that the role of an exchange field in superconductors is played by the chemical potential  $\mu_{1,2}$ . However, the *independent* tunability of the hopping integral  $t_{1,2}$  (or the effective bandwidth) within each layer has no counterpart in the case of superconductors. We note that the parameters  $t_{1,2}$  are related to the effective mass  $m_{1,2}$  appearing in the continuum limit.<sup>18,19</sup> When  $\xi_{\mathbf{k},1} = -\xi_{\mathbf{k},2}$ , the first term on the rhs disappears, while the first term in the square root is maximized. The quasiparticles are fully gapped, suggesting the “quenched” uniform state with zero-momentum pairing is a truly favored state. However, when  $\xi_{\mathbf{k},1} \neq -\xi_{\mathbf{k},2}$ , there emerges an instability toward a *finite*-momentum pairing state. This analysis is consistent with that given in Refs. 18 and 19 and will be corroborated by the numerical calculations presented below.

In our numerical calculations, we choose to measure all energy quantities in units of the hopping integral for the electron layer and set  $t_1 = 1$ . The Boltzmann constant is set to  $k_B = 1$ . A typical system size of  $N_L = 24 \times 24$  is used throughout the calculation and the convergence criterion, set as the difference between two consecutive iterations, is no larger than  $3 \times 10^{-5}$ . For the convenience of discussion, we introduce the average chemical potential and pseudospin polarization potential as  $\mu = (\mu_1 - \mu_2)/2$  and  $h = (\mu_1 + \mu_2)/2$ , and the degree of bandwidth mismatch  $\alpha = -t_2/t_1$ . Without loss of generality, we take  $\alpha = 1$  throughout this work.

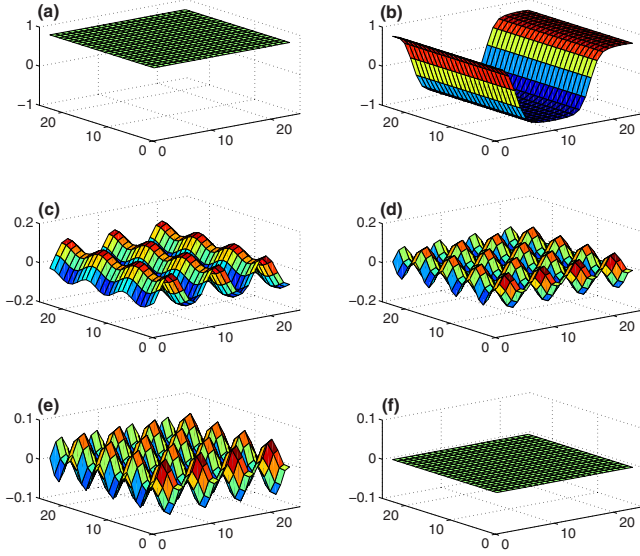


FIG. 3. (Color online) The spatial dependence of the exciton order parameter for changing  $h=0$  (a), 0.2 (b), 0.6 (c), 0.7 (d), 1.0 (e), and 1.60. The temperature is chosen as  $T=10^{-3}$ . The average chemical potential is chosen as  $\mu=-0.5$ .

#### A. Spatial dependence of the order parameter and phase diagram

In Fig. 3, we show the order-parameter texture on a square lattice for varying polarization field strength,  $h$ , at fixed values of  $\mu=-0.50$  and  $g_0=3$ . When the polarization degree of freedom  $h=0$ , the exciton order parameter is uniform [see Fig. 3(a)]. As  $h$  deviates from zero, the order parameter first exhibits a one-dimensional modulation [see Fig. 3(b)]. In this regime, the order parameter changes sign across the nodal lines. Our numerical calculations demonstrates (not shown) that the sign-change slope becomes steeper as the pairing strength is increased such that the nodal lines are replaced by sharp domain walls—a manifestation of a BCS-BEC crossover. We note that the formation of domain walls has also been obtained in the context of superconductors<sup>21–26</sup> and resonant Fermi gas<sup>27</sup> for either weak exchange field or small density imbalance. With increased polarization, the modulation periodicity is shortened, and the one-dimensional modulation gives way to a two-dimensional one [see Figs. 3(c)–3(e)]. Simultaneously, the amplitude of the order parameter is decreased. Ultimately, the system enters a polarized normal state with even larger  $h$  [see Fig. 3(f)]. Our calculations find that the LO-like state, which breaks the translational symmetry of the underlying lattice, is always favorable.

In Fig. 4, we provide a schematic of the typical  $\mu$ - $h$  phase diagram for the electron-hole bilayer defined on a square lattice. The phase diagram is constructed with delineating lines  $\mu+h=\pm 4$  and  $-\mu+h=\pm 4$ . For  $\mu+h<-4$ , there are no electrons occupying the electron band while for  $\mu+h>4$ , the electron band is fully occupied by electrons. Similarly, for  $-\mu+h<-4$ , the hole band is fully occupied, while for  $-\mu+h>4$  the hole band is empty. In this way, we can map out the normal-state phases, including a zero occupation phase (ZZ), full occupation phase (FF), a phase with one of

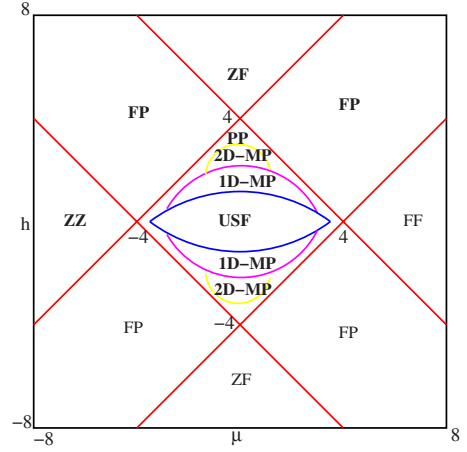


FIG. 4. (Color online) Schematic of the electron-hole bilayer phase diagram, covering three superfluid phases (USF, 1D-MP, and 2D-MP), and several normal phases (ZZ, FF, ZF, FP, and PP).

the layers fully occupied with the other empty (ZF), a fully polarized phase with partial occupation of only one type of carrier in the respective layer (FP), and a partially polarized phase (PP). The interesting exciton phases are limited to the area bounded by the aforementioned four delineating lines. They are categorized into a BCS (or BEC) uniform superfluid (USF) phase, and one-dimensional (1D) and two-dimensional (2D) modulated phases (MPs).

#### B. Local electronic structure in the LO phase

The inhomogeneous exciton state has physical implications. We calculate the average local density of states for the electron and hole layers,

$$\rho_e(E) = \frac{1}{N_L} \sum_{i,n} |u_i^n|^2 \delta(E - E_n), \quad (8a)$$

$$\rho_h(E) = \frac{1}{N_L} \sum_{i,n} |v_i^n|^2 \delta(E + E_n). \quad (8b)$$

The Dirac  $\delta$  function in the above equations is approximated by a Lorentzian  $\delta(E - E_n) \rightarrow (\gamma/\pi)[(E - E_n)^2 + \gamma^2]^{-1}$  with  $\gamma=0.02$ . In the numerical calculation, we have also used a supercell technique to partially remove the finite-size effect. In Fig. 5, we show the average local density of states for various values of the polarization strength  $h$ . When  $h=0$  [see Fig. 5(a)], the LDOS exhibits a standard BCS-like quasiparticle gap around zero energy since the exciton condensate is uniform [corresponding to Fig. 3(a)]. In this phase, the quasiparticle density of states are identical for the electron and hole layers. When  $h$  is small but finite, for which the system is in the 1D exciton modulated state [corresponding to Fig. 3(b)], the density of states exhibits resonance peaks within the BCS-like gap [see Fig. 5(b)]. An equal number of such resonance peaks appear in the density of states for the electron and hole layers, respectively. The origin of these resonance peaks are related to the Andreev-type reflection, which is responsible for the bound-state formation in the supercon-

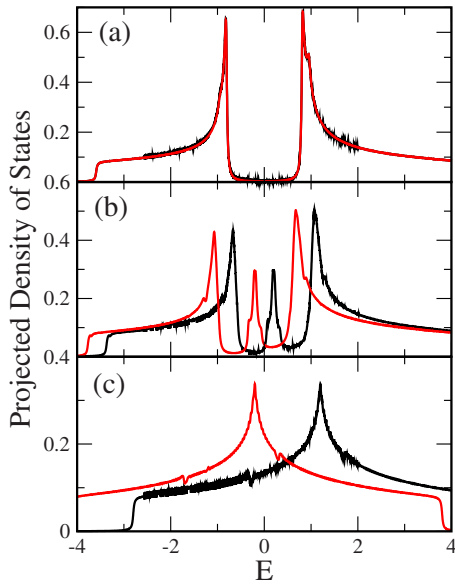


FIG. 5. (Color online) Average projected density of states for electron (black-solid line) and hole (red-dashed line) layers at various values of  $h=0$  (a),  $0.2$  (b), and  $0.7$  (c). The average chemical potential  $\mu=-0.5$ .

ducting junctions with a  $\pi$  phase shift.<sup>28</sup> We notice that in the BEC limit, multiple peaks can appear in the projected density of states. In addition, since the density is imbalanced (for nonzero  $h$ ), the overall density-of-states spectrum is shifted in opposite directions for the electron and hole layers. When  $h$  is further increased [see Fig. 5(c)], the shift of the overall density-of-states spectrum is increased for the electron and hole layers, and the quasiparticle gap structure becomes invisible because the exciton order parameter has been significantly suppressed [corresponding to Fig. 3(d)].

To understand the nature of the quasiparticle peaks exhibited in the density of states for the 1D modulated state, we present in Fig. 6 the spatial variation of the local density of states at the resonance energies. It can be seen that the local density of states at these energies has a maximum at the nodal lines and shows an exponential-like decaying behavior, indicating that these states are bound states.

#### IV. SUMMARY

We have studied the texture of the exciton condensate at low temperatures in two parallel and independently gated electron-hole layers by solving a microscopic model Hamil-

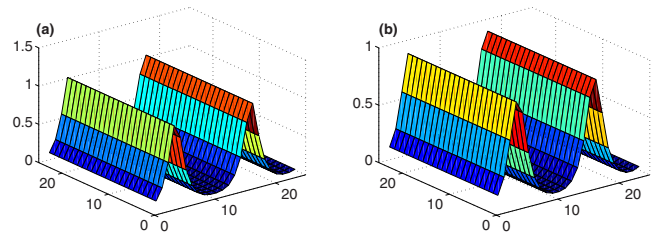


FIG. 6. (Color online) Spatial variation of the local density of states at (a)  $E=0.184$  and (b)  $-0.190$ , corresponding to the intragap peaks shown in Fig. 5(b).

tonian in real space at a mean-field level. We have found that, with increased density imbalance, the system experiences transformations from the zero center-of-mass momentum superfluid state, through one- and two-dimensional exciton pair modulated states, into the normal state. At weak density polarization, the modulated state resembles the Larkin-Ovchinnikov state in superconductors in the presence of an exchange field in the weak-coupling BCS limit, and becomes stripe-like in the strong-coupling BEC limit. In this phase, the density of states exhibits low-energy intragap resonance peaks. A local-density-of-states imaging analysis indicates that these peaks correspond to bound state pinned near the nodal lines. Since the local density of states is proportional to the differential tunneling conductance as measured by scanning tunneling spectroscopy/microscopy, the inhomogeneous exciton modulated state should be experimentally accessible.<sup>29</sup> Therefore, an electron-hole bilayer system with density imbalance controlled by gate voltage, can provide an alternative setting for testing exotic phases proposed in superconductors.

A remark is in order: we notice that our phase diagram, as shown in Fig. 4, is obtained with a contact electron-hole pairing interaction, where the LO-like modulated phases occupy a reasonable size of the region. A more recent work<sup>30</sup> has studied the effects of intralayer interaction and Coulomb screening on the superfluid mass density, and has indicated that the FFLO-like superfluid phase can be stabilized by the screening interaction with the phase region reduced by switching on the intralayer interactions.

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