Nanotechnology-Driven Engineered Materials

New Insights

Editors

Sabu Thomas | Yves Grohens Nandakumar Kalarikkal | Oluwatobi Samuel Oluwafemi Praveen K. M.





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NANOTECHNOLOGY-DRIVEN ENGINEERED MATERIALS

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Edited by

Sabu Thomas, PhD Yves Grohens, PhD Nandakumar Kalarikkal, PhD Oluwatobi Samuel Oluwafemi, PhD Praveen K. M. Author Copy



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CHAPTER 6

ELECTRON–HOLE BILAYER SYSTEMS IN SEMICONDUTORS: A THEORETICAL PERSPECTIVE

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ABSTRACT

In this generation of semiconductor-based miniature gadgets, it is always an intriguing issue to understand the underlying mechanism of these highly sophisticated devices. Systematic exploration uncovers the fascinating world of nano-scale physics; however, a deeper probe actually unearths the salient nature of electron-hole interaction which is the soul of semiconductor physics. In this essay, we plan to shed some light on the interplay of different interactions in electron-hole systems. This study is purely theoretical; however, we put forward recent experimental successes at suitable places. Here, we explicate the intricacies involving electron(hole)-electron(hole) and electron-hole interaction in the realm of mean-field theory. To make our description more comprehensive and complete, we elaborate the theoretical analysis by means of both path integral formalism and canonical transformation method. The discussion clearly suggests that the interplay of intra-layer and inter-layer interactions results in the formation of several exotic phases such as Sharma phase and Fulde-Ferrell-Larkin-Ovchinniov (FFLO) phase.

6.1 INTRODUCTION

The last century, widely believed as the century of physics, has witnessed several experimental and theoretical accomplishments in condensed matter physics and optics, which has paved the way for future industrial revolution in communication and computation. There was an enormous jump in terms technology when vacuum diodes were replaced by semiconductor transistors, but that was a good 60 years back. As we are exhausting the ceiling of the Moore's Law,¹ it is now evident that we need to try something different while keeping the flavor of our old prodigy (semiconductor physics).

The emergence of ultra-cold atom research in the last decade,²⁻¹⁰ has widened the possibility to study different exotic phases of matter by controlling the interaction. The smooth transition of Cooper pairs from BCS superconductors to Bose superfluid of composite bosons for trapped atoms is one of such developments. This phenomenon is known as Bardeen-Cooper-Schrieffer–Bose-Einstein-Condensate (BCS–BEC) crossover. Although trapped atoms represent an ideal testing ground for a fundamental understanding of the BCS–BEC crossover, technological applications exploiting the occurrence of condensates will most probably

rely on semiconductor systems. In these systems, excitons, made up of electrons and holes, play the role of composite bosons.¹¹ Formation of excitons between spatially separated electrons and holes and their subsequent condensation have long been predicted and arguably observed nearly 30 years later experimentally.¹²

The main objective of this chapter is to provide a comprehensive theoretical guide to deal with electron-hole (e–h) systems in the mean-field level. We start with a brief description of BCS–BEC crossover in ultracold atomic gases, excitonic systems, and the meaning of crossover in e–h systems. Usually, an exitonic system is modeled by taking into account their inter- and intra-species interactions. Here we first elaborate the system in the absence of intra-layer interaction and later incorporate it. However, for a better theoretical view, we employ two different mathematical techniques, namely path integral formalism and canonical transformation, in our discussion. At the fag end, we briefly comment on the possible way to include impurity in these systems. We conclude with current experimental status in this field with possible future applications.

6.1.1 BCS-BEC CROSSOVER

The experimental realization of Bose-Einstein condensate in trapped ultra-cold alkali gases^{13,14} appeared as a new ray of light to the science community. For its broad appeal, people from diverse communities of physics, such as atomic and molecular physics, condensed matter physics, and nuclear physics, came under a single umbrella. The excitement led to the study of both bosonic and fermionic gases. Further, the application of Fano-Feshbach resonance (which we will discuss later)^{15–17} in atomic gases^{18–21} gave freedom to evolve a composite boson state to Cooper pairs passing the crossover.

In normal superconductors, electrons with opposite spins pair to form Cooper pairs below the superconducting critical temperature. The average pair size ξ_{pair} for these superconductors is much larger than the mean interparticle distance k_F^{-1} . Therefore, the quantity $\xi_{pair}k_F$ is much larger than 1. So the Cooper pairs are largely overlapping and it is not appropriate to consider them as spin-zero bosons. It is better to appreciate them as correlation of two opposite spin fermions at a certain distance and BCS theory holds for them perfectly. But the advent of high-temperature superconductor, where $\xi_{nair}k_F$ is of the order 5–10, forced to think beyond the BCS theory. The coupling between the fermions in these novel superconductors suggests an intermediate state between Cooper pairs and composite bosons. This intuitive idea prompted to develop a theory which can connect both the BCS theory for Cooper pairs and BEC for composite bosons. Already at that time, there were some works^{23–25} where the evolution of the fermionic pairs from Cooper pairs to composite bosons had been studied. Since the transition between these two limits occurs without an intermediate phase transition, the phenomenon has referred as BCS–BEC crossover. Figure 6.1 gives a physical feeling of the situation where densely packed Cooper pairs and sparsely distributed composite bosons are on both sides and in between there exist the strongly interacting fermionic pairs which are the main players in the crossover. Subsequent to the discovery of the high temperature superconductors, the interest in the crossover physics has surged.²⁶⁻³¹



The beauty of the BCS ground state is that it not only describes the superconductivity pretty efficiently but also contains the essence of the bosonic limit. If one starts from the BCS ground state wave function $|\Psi\rangle$ and carries out the necessary algebraic rearrangements in the following manner,

$$|\tilde{\Psi}\rangle = \prod_{k} (u_{k} + v_{k}c_{k\uparrow}^{\dagger}c_{-k\downarrow}^{\dagger})|0\rangle$$
$$= \prod_{k} u_{k}(1 + \frac{v_{k}}{u_{k}}c_{k\uparrow}^{\dagger}c_{-k\downarrow}^{\dagger})$$
(6.1)
For No_E $u_{k}e^{\sum_{k} g_{k\uparrow}c_{k\uparrow}^{\dagger}c_{-k\downarrow}^{\dagger}}|0\rangle$, ial Use

then one can define the operator $b^{\dagger} = \sum_{k} g(k) c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger}$, which contains fermionic pairs. However the defined operator can not be regarded as a true bosonic operator because,

$$[b,b] = \sum_{k} |g(k)|^{2} (1 - n_{k\uparrow} - n_{-k\downarrow} \neq c \quad \text{number.}$$
(6.2)

In certain conditions when $\langle n_{k,\sigma} \rangle \langle \langle 1, [b, b^{\dagger}] \rangle \simeq 1$, the *b* turns out truly a bosonic operator and in that situation,

$$|\tilde{\Psi}\rangle = \exp(b^{\dagger})|0\rangle \tag{6.3}$$

represents a bosonic coherent state or a condensate.²³⁻²⁵

The simplest description of the BCS–BEC crossover can be given at the mean-field level for a homogeneous system in the zero temperature limit. In this situation, it is necessary to analyze a pair of coupled equation which reads,

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \left(\frac{1}{2E_k} - \frac{m}{k^2} \right) = -\frac{m}{4\pi a_F}$$

$$\int \frac{d\mathbf{k}}{(2\pi)^3} \left(1 - \frac{\xi_k}{E_k} \right) = n$$
(6.5)

where the notations are the usual BCS notations. Precisely, $\xi_k = k^2/2m - \mu$, $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ and the bare coupling strength has been replaced by the s-wave scattering length. And eq (6.4) is known as gap equation and eq (6.5) is known as density equation. The original gap equation actually contains an ultraviolet divergence (originated from the assumption that the contact potential governs fermionic interaction); however, here the equation is suitably regularized to avoid the mentioned divergence. The coupled equations can be solved simultaneously for a given density and coupling. These solutions are plotted in Figure 6.2 where we have evaluated the pairing gap (Δ) and chemical potential (μ). In describing the chemical potential, two different normalizations are adopted depending on the sign of the chemical potential. When $\mu > 0$, it has been normalized by the Fermi energy ($\epsilon_p = k_F^2/2m$) and in the negative side we used two body binding energy ($\epsilon_0 = (ma_F^2)^{-1}$) to normalize.



FIGURE 6.2 Variation of order parameter (pairing gap) and chemical potential with coupling strength in a homogeneous system.

6.1.2 EXCITONS

The manifestation of BEC is based on the wave nature of particles. Therefore, it is obvious that de Broglie hypothesis plays a crucial role in understanding the condensate. It can be shown that the de Broglie wavelength gets longer with decrease in temperature. When atoms are cooled to the point where the thermal de Broglie wavelength is comparable to the inter-atomic separation then BEC formation actually starts. The relation between the transition temperature and peak atomic density (n) can be estimated as $n\lambda_{dB}^3 = 2.612$ where the de Broglie wavelength (λ_{dB}) is defined as $\lambda_{dB} = h/mv = h/\sqrt{mk_BT}$, where *m* is the mass of the atom, k_B is the Boltzmann constant, and T is the temperature. The critical temperature for the transition works out in the range of nano-Kelvin. The above description also points out that the de Broglie wavelength is inversely proportional to the square-root of the mass of the particle. Therefore, it took a long time to develop the necessary cooling techniques to create BEC with heavy atomic mass. For solid-state systems, excitons in semiconductors have long been considered as a promising candidate for BEC because of their light mass as compared to the neutral atoms. Usually, effective mass of exciton is considered as twice the mass of electron. Now if we employ this mass in the de Broglie theory, the critical temperature for transition in two dimension turns out about 1K. The possibility of achieving higher critical temperature in excitonic systems infuses additional interest in the research community. Unfortunately, excitons recombine quickly, too fast to allow a condensate to form. Although excitons coupled to light confined within a microcavity can form hybrid particles that do live long enough to

condense, such condensates require a continuous input of light.³² This is known as exiton-polariton condensate which has actually been observed very recently.³³ However, a very recent study based on two mono-layers of graphene separated by an insulating material poses promising platform to realize excitonic condensate.^{34,35}

Excitons can be defined as a bound state of an electron and hole which are attracted to each other by the electrostatic Coulomb force. It is an electrically neutral quasiparticle that exists in insulators, semiconductors, and in some liquids. An exciton can form when a photon is absorbed by a semiconductor. This excites an electron from the valence band into the conduction band. In turn, this leaves behind a localized positively charged hole. The electron in the conduction band is then attracted to this localized hole by the Coulomb force. This attraction provides a stabilizing energy balance. The recombination of the electron and hole, that is, the decay of the exciton, is limited by resonance stabilization due to the overlap of the electron and hole wave functions, resulting in an extended lifetime for the exciton.

6.2 BCS–BEC CROSSOVER WITH EXCITONS

As mentioned earlier, electronic systems in semiconductor devices provide an alternative and technically more viable route for physical realization where BCS-BEC crossover. Electrons and holes can form bound states due to the attractive Coulomb interaction between them. These bound states are popularly known as excitons. Thus excitons are the composite bosons in this system. The interaction strength can be changed by varying the density. Here, we must note that in ultra-cold atomic systems, the controlling parameter is either s-wave scattering length or the density, whereas in semiconductor systems, it is only the density or the concentration of electrons and holes. Another significant difference from usual unitary Fermi gas is that the most commonly used interaction in those systems is short-range contact interaction, whereas in semiconductors, it is usually long-range Coulomb interaction. The long-range ordering due to Coulomb interaction complicates the emergence of condensate in the excitonic systems. Of late, several theoretical ideas have been floated to tackle this problem. 36-39ON-COMMERCIAL USE

However, the condensation phenomenon of excitons is a fairly old issue. It was first predicted almost 50 years before by Blatt et al.⁴⁰ In the

early 1980s, Comte et al. studied the Bose condensed ground state of an electron–hole gas in a simple model semiconductor, as a function of density, using a mean field variational ansatz.^{41,42} Later with the advent of new technologies and experimental observation of weakly interacting BEC, the research on excitonic condensate received a new impetus. A keen interest is paid to the bilayer quantum-well systems realized in semiconductor hetero-structures. In recent years, using electrical and optical techniques exciton condensation has been observed in several different systems. Quantum Hall experiments at half-filling investigate BEC in electron–electron and hole–hole bilayers.^{11,43,44} Optically generated bilayer excitons also show evidence for condensation.¹² Recently, excitons coupled to photons to form polaritons with even smaller mass leading to higher condensation temperatures have been studied theoretically⁴⁵ and experimentally.^{46,47}

6.2.1 THEORY OF EXCITONS

The first theoretical mean-field analysis of excitons can be found in [Refs.41 and 42] However, they involved equal electron and hole densities leading to full pairing. In recent years Pieri et al. extended the abovementioned pioneering works for density imbalance.⁴⁸ The investigation reveals a crossover in the phase diagram from the BCS limit of overlapping pairs to the BEC limit of non-overlapping tightly bound pairs. Further, it was noted that different novel phases emerge in the crossover region when the densities of electrons and holes are varied independently. However, this analysis only takes into account the inter-layer Coulomb interaction between the electrons and holes, thereby it neglected the intralayer electron–electron and hole–hole Coulomb interactions. Later Subasi et al. overcame this deficiency.⁴⁹ Hence a typical bilayer Hamiltonian in the mean-field level consists of a kinetic energy/hopping term, intra-layer interaction term, and inter-layer interaction as described in eq (6.6).

$$H = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}}^{a} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \epsilon_{\mathbf{k}}^{b} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}) + \frac{1}{2V} \sum_{\mathbf{k}_{1}, \mathbf{k}_{2}, \mathbf{q}} U_{\mathbf{q}}^{aa} a_{\mathbf{k}_{1}+\mathbf{q}}^{\dagger} a_{\mathbf{k}_{2}-\mathbf{q}}^{\dagger} a_{\mathbf{k}_{2}} a_{\mathbf{k}_{1}} + \frac{1}{2V} \sum_{\mathbf{k}_{1}, \mathbf{k}_{2}, \mathbf{q}} U_{\mathbf{q}}^{ab} a_{\mathbf{k}_{1}+\mathbf{q}}^{\dagger} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{1}+\mathbf{q}}^{\dagger} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{1}+\mathbf{q}}^{\dagger} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{1}+\mathbf{q}}^{\dagger} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{1}+\mathbf{q}}^{\dagger} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{1}+\mathbf{q}}^{bb} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{2}}^{bb} b_{\mathbf{k}_{1}+\mathbf{q}}^{bb} b_{\mathbf{k}_{2}-\mathbf{q}}^{bb} b_{\mathbf{k}_{2}-\mathbf{q}}^{b} b_{\mathbf{k}_{2}-\mathbf{q}}^{b} b_{\mathbf{k}_{2}-\mathbf{q}}^{b$$

The basis states for electrons and holes are chosen to be plane wave states. The operators $a_k / a_k^{\dagger}(b_k / b_k^{\dagger})$ are creation and annihilation operators for electrons and holes, respectively. The single particle energies are denoted by \in_k^a, \in_k^b , and the matrix element U_q with respect to plane wave states becomes the Fourier transform of the corresponding two-body interaction,

$$U_{q} = \int e^{-iq \cdot r} U(r) dr.$$
 (6.7)

In eq (6.7), U^{aa} , U^{bb} , and U^{ab} denote electron–electron, holehole, and electron–hole Coulomb interactions, respectively. The explicit forms of the Coulomb potentials can be noted as,

$$U_q^{aa} = U_q^{bb} = \frac{2\pi e^2}{\epsilon q}, \qquad U_q^{ab} = \frac{2\pi e^2}{\epsilon q} e^{-qd}, \qquad (6.8)$$

where d denotes the distance of separation between electron and hole layers.

Here, we plan to elaborate the discussion in the following manner. First we will explain the bilayer systems in the light of only the inter-layer interaction (i.e., $U^{aa} = U^{bb} = 0$).⁴⁸ Later we will move forward and include the intra-layer interaction.⁴⁹

6.2.1.1 IN ABSENCE OF INTRA-LAYER INTERACTION

If we neglect the intra-layer interaction for the time being, eq (6.6) can be rewritten as,

$$H = \sum_{k} (\in_{k}^{a} a_{k}^{\dagger} a_{k} + \in_{k}^{b} b_{k}^{\dagger} b_{k}) + \sum_{k} (\Delta_{k} a_{k}^{\dagger} a_{-k}^{\dagger} + \Delta_{k}^{*} b_{-k} a_{k}).$$
(6.9)

Here $\Delta_k = -\sum_{k'} U_{kk'}^{ab} \langle a_{k'} b_{-k'} \rangle$ and $\in_k^a = \hbar^2 k^2 / 2m_b$, where *a* and *b* denote the electron and hole respectively.

Now eq (6.9) can be analyzed by using path integral formulation as well as canonical transformation. However, here we plan to explicate the path integral formalism at first and in the latter half (with intra-layer interaction) we will explain the canonical transformation. This will enable the readers to view the bilayer problem through two different mathematical angles, albeit both the cases are akin to each other.

6.2.1.2 PATH INTEGRAL FORMALISM

The path integral formalism deduced here is constructed in analogy with the BCS theory. However, compared to the BCS theory, the single particle energies are not equal to each other (i.e., $\in_k^a \neq \in_k^b$) due to the difference in electron and hole mass. Let us now introduce the chemical potential (μ) in the mean-field Hamiltonian which will ensure the density imbalance. Hence eq (6.9) reads,

$$H - \mu N = \sum_{k,\sigma} \epsilon_k^{\sigma} \sigma_k^{\dagger} \sigma_k - \mu^{\sigma} \sigma_k^{\dagger} \sigma_k + \sum_k [\Delta_k a_k^{\dagger} b_{-k}^{\dagger} + \Delta_k^{\ast} b_{-k} a_k]$$

$$= \sum_{k,\sigma} \xi_k^{\sigma} \sigma_k^{\dagger} \sigma_k + \sum_k [\Delta_k a_k^{\dagger} b_{-k}^{\dagger} + \Delta_k^{\ast} b_{-k} a_k],$$

(6.10)

where $\sigma \in \{a, b\}$ and $\xi_k = \epsilon_k - \mu$. Hence the quantum partition function in path integral form can be written as, $Z = \int D[\Delta, \overline{\Delta}] e^{-S_{eff}}$ where,

$$S_{eff} = \int d^3x \int_0^\beta d\tau \left[\frac{\Delta \overline{\Delta}}{U} - \operatorname{Tr} \ln G^{-1}\right].$$
 (6.11)

 $G^{-1} \text{ is defined as Nambu propagator (inverse Greens function). The Greens function contains the free particle Green's function <math>(G_0^{-1})$ and the particleparticle interaction incorporated through self-energy (Σ). Thus $G^{-1} = G_0^{-1} + \Sigma$. Since the thermodynamic potential can be expressed as $\Omega = -\frac{\ln Z}{\beta}$ and density as $n = -\frac{\partial \Omega}{\partial \mu}$, therefore a careful analysis of eq (6.11) leads to $\mathbf{n}_i = \frac{1}{\beta} \frac{\partial}{\partial \mu_i} \ln \int D[\Delta, \overline{\Delta}] \left[\exp\left\{ -\int d^3 x \int_0^\beta d\tau \left(\frac{\Delta \overline{\Delta}}{U_{ab}} - \operatorname{Tr} \ln G^{-1} \right) \right\} \right]$ $= \frac{1}{\beta} \frac{\partial}{\partial \mu_i} \ln \left[\exp\left\{ \sum_{k,i\omega} \operatorname{Tr} \ln G^{-1}(k,i\omega) \int D[\Delta, \overline{\Delta}] \exp\left[-\frac{V\beta\Delta, \overline{\Delta}}{U} \right] \right\} \right]$ (6.12) $= \frac{1}{\beta} \sum_{k,i\omega} \operatorname{Tr} \left[G \frac{\partial}{\partial \mu_i} G^{-1} \right]$

where the suffix, $i \in \{a, b\}$, the $\int D[\Delta \overline{\Delta}]$ integral reduces to 1 through Grassmann identity. The explicit definition of the Green's function can be noted as follows, **NON-COMMERCIALUSE**

$$G^{-1} = \begin{pmatrix} i\omega + \xi_{k}^{b} & \Delta_{k} \\ \overline{\Delta}_{k} & i\omega - \xi_{k}^{a} \end{pmatrix} \text{ and } G = \begin{pmatrix} \frac{i\omega - \xi_{k}^{a}}{D} & \frac{\Delta_{k}}{D} \\ \frac{\overline{\Delta}_{k}}{D} & \frac{i\omega - \xi_{k}^{b}}{D} \end{pmatrix}$$

where, $D = -\omega^{2} - i\omega(\xi_{k}^{a} - \xi_{k}^{b}) - \xi_{k}^{a}\xi_{k}^{b} - \Delta_{k}^{2}$. Hence, from eq (6.12),
$$n_{a} = \frac{1}{V\beta} \sum_{k,i\omega} \operatorname{Tr} \left(\frac{i\omega - \xi_{k}^{a}}{D} & \frac{\Delta_{k}}{D} \\ \frac{\overline{\Delta}_{k}}{D} & \frac{i\omega - \xi_{k}^{b}}{D} \right) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
$$= \frac{1}{V\beta} \sum_{k,i\omega} \frac{i\omega + \xi_{k}^{b}}{D}.$$
(6.13)

D can be decomposed in a factorized form as follows, $D = (i\omega - \Delta \xi_k - E_k)$ $(i\omega - \Delta \xi_k + E_k) = (i\omega - E^+)(i\omega + E^-)$. We carry out the Matsubara frequency sum from eq (6.13) as,

$$n_{a} = \frac{1}{V} \frac{1}{\beta} \sum_{k,i\omega} \frac{i\omega + \xi_{k}^{b}}{i\omega - E^{+})(i\omega + E^{-})} f(i\omega)$$

$$= \frac{1}{2V} \sum_{k} \left[\left(1 + \frac{\xi_{k}}{E_{k}} \right) f_{k}^{+} + \left(1 - \frac{\xi_{k}}{E_{k}} \right) (1 - f_{k}^{-}) \right].$$
(6.14)

In a similar fashion we can also evaluate n_b as,

$$n_{b} = \frac{1}{2V} \sum_{k} \left[\left(1 + \frac{\xi_{k}}{E_{k}} \right) f_{k}^{-} + \left(1 - \frac{\xi_{k}}{E_{k}} \right) (1 - f_{k}^{+}) \right].$$
(6.15)

Here f(E) is defined as the Fermi function at zero temperature and

$$f_{k}^{\pm} = \begin{cases} 1 & \text{if } E_{k}^{\pm} < 0 \\ 0 & \text{if } E_{k}^{\pm} > 0 \end{cases}$$
$$E_{k}^{\pm} = E_{k} \pm \Delta \xi_{k}$$
$$\Delta \xi_{k} = \frac{1}{2} (\epsilon_{k}^{a} - \mu_{a} - \epsilon_{k}^{b} - \mu_{b}).$$

The other relevant equation known as gap equation can also be derived from the effective action as, Commercial Use

$$S_{eff}\left[\Delta,\overline{\Delta}\right] = \int d^{3}x \int_{0}^{\beta} d\tau \left[\frac{\Delta \overline{\Delta}}{U_{ab}} - \operatorname{Tr}\ln\left(-G^{-1}\right)\right]$$
$$= \frac{V\beta \Delta \overline{\Delta}}{U_{kk'}} - \ln\prod_{k}\left|-G^{-1}\right|.$$

It can be shown that $|-G^{-1}| = D$, where *D* is same as defined earlier. One can also write, $\ln \prod_k \simeq \sum_k \ln$. Hence,

$$S_{eff}\left[\Delta,\overline{\Delta}\right] = \beta V \frac{\Delta \overline{\Delta}}{U_{kk'}} - \sum_{k,i\omega} \ln D$$
(6.16)

Applying the saddle point approximation $\frac{\delta S_{eff}}{\delta \overline{\Delta}} = 0$, we can rewrite eq. (6.16) as

$$\frac{V \beta \Delta_{k}}{U_{kk'}} - \sum_{k,i\omega} \frac{\Delta}{D} = 0$$

$$\frac{V \Delta_{k}}{U_{kk'}} = \frac{1}{\beta} \sum_{k',i\omega} \frac{\Delta_{k'}}{(i\omega - E^{+})(i\omega + E^{-})} f(i\omega)$$

$$= \sum_{k'} \frac{\Delta_{k'}}{2E_{k'}} \Big[f^{+} - (1 - f^{-}) \Big]$$

$$= -\frac{1}{V} \sum_{k'} U_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \Big[1 - f_{k'}^{+} - f_{k'}^{-} \Big].$$
(6.17)

One can now solve eqs (6.14),(6.15), and (6.17) self-consistently to study the effect of density imbalance. However, before elaborating the obtained results of Ref. [48], it is important to discuss the units of the observables. All through this discussion, the physical quantities are in Rydberg units, that is, length is measured in effective (excitonic) Bohr radius $a_B = \frac{\hbar^2 \varepsilon}{me^2}$, momentum in $1/a_B$, and energy in effective Rydberg ($\text{Ryd} = \frac{\hbar^2}{2ma_B^2} = \frac{e^2}{2\varepsilon a_B}$). The reduced mass *m* is defined as $1/m = 1/m_a + 1/m_b$ where $m_a = m_e$ and $m_b = m_h$ are the band mass of the electron and hole, respectively. As mentioned before, the bilayer system is characterized by the electron– hole densities or by the average density parameter (r_s) and population polarization (α). α signifies the population imbalance and is defined as the ratio of density difference and total density. In other words, r_s and α can be described as,

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Electron-Hole Bilayer Systems in Semicondutors

$$n = \frac{n_a + n_b}{2} = \frac{1}{a_b^2 r_s^2}$$
 and $\alpha = \frac{n_a - n_b}{n_a + n_b}$ (6.18)

The BCS and BEC regimes are defined by means of average inter-particle spacing, that is, $r_s < 1$ implies closely packed systems thereby it is noted as BCS regime. Otherwise when $r_s > 1$, it is considered as BEC regime. By solving the coupled density and gap equation it is possible to study the smooth transition of the physical observables from one region to another region. Hence, we can borrow the BCS–BEC crossover analogy from ultra-cold atomic systems to the semiconductor systems without losing much of the generality.

Self-consistent analysis of eqs (6.14), (6.15), and (6.17) results in evaluation of the gap function. In Figure 6.3a, the wave-vector dependence of gap function is depicted. One can observe that at low r_s (BCS regime), there exists a distinct peak for the gap function; however, this peak smoother out as we increase the average inter-particle distance, that is, we move from highly overlapping BCS system to non-overlapping BEC system. Similar density-induced BCS–BEC crossover had already been studied in ultracold atomic systems.^{53,54} Figure 6.3b describes the maximum value of the gap function for different densities with varying degree of imbalance. Here we observe that the maximum value exists at about zero average chemical potential ($\mu = (\mu_e + \mu_h)/2$). This actually implies a robust paradigm of superfluidity in the crossover region. Interestingly, this conclusion was also made from the perspective of ultra-cold clean Fermi gases⁵³ and dirty Fermi gases.⁵³ One can also notice that the magnitude of the energy gap actually reduces with increase in density imbalance.



FIGURE 6.3 (a) The dependence of wave vector on gap function as balanced density $(\alpha = 0)$ at various values of r_s . (b) Variation of $max{\Delta_k}$ at different imbalances and different densities. For both the figures the inter-layer separation was considered as unity (d = 1). (Reprinted Ref [51] with permission from the author.)

Figure 6.4 shows the zero-temperature phase diagram for d = 1. We can identify various phases using Δ_k , determined from eq (6.17), and the superfluid density ρ_s . Within mean-field theory at $T = 0 \rho_s$ is defined as,

$$\rho_{s} = m_{e}n_{e} + m_{h}n_{h} - \frac{1}{4\pi} \sum_{j,\lambda} \frac{\left(k_{j}^{\lambda}\right)^{3}}{\left|\frac{dE_{k}^{\lambda}}{dk}\right|_{k=k_{j}^{\lambda}}}$$
(6.19)

Here, k_j^{λ} is the *j*-th zero of $E_k^{\lambda} = 0$ with $\lambda = (+, -)$. The zeros of quasiparticle energies, E_k^+ (E_k^-), can be found only for imbalanced density scenario while no zero occurs for $\alpha = 0$.

The normal phase (N) corresponds to the trivial solution $\Delta_k = 0$. The Sarma phases corresponds to nonvanishing Δ_k when $a \neq 0$ and positive superfluid density ρ_s . The S1 and S2 denote the Sarma phases for one and two Fermi surfaces, respectively. There will be one zero of E_k^{λ} (j = 1) for the S1 phase (one Fermi surface) and two zeros (j = 1, 2) for the S2 phase (two Fermi surfaces). A negative value of ρ_s in eq (6.19) indicates that the Sarma phase is unstable toward a phase with a spontaneously generated superfluid current, which we associate with the Fulde–Ferrell–Larkin–Ovchinniov (FFLO) phase.^{56,57}

One intriguing aspect of Figure 6.4 is the dependence of the phase diagram on the sign of α . In particular, while the boundary of the normal phase does not depend appreciably on the sign of α , the region of stability of the Sarma phase with respect to the FFLO phase depends dramatically on the sign. For $\alpha < 0$, the phase diagram is dominated by the FFLO phase, with the S1 phase being confined to the extreme BEC region, while for $\alpha > 0$, the FFLO phase is compressed into the region of small r_s .



FIGURE 6.4 Zero temperature phase diagram for d = 1. The dashed line indicates $\mu = 0$ and the dashed dotted line indicates the separation between S1 and S2 phases.⁵¹

Electron-Hole Bilayer Systems in Semicondutors

6.2.1.3 CANONICAL TRANSFORMATIONS

We can now introduce an extra complexity in the system, namely the intralayer interaction, to explore further. However, for a transparent understanding of the mean-field formalism here we will follow the canonical transformation method to obtain the necessary mean-field equations. Our starting point is again eq (6.6) and now $U_q^{aa} = U_q^{bb} \neq 0$. One can now apply Bogoliubov transformation with operators α_k^{\dagger} and β_{-k}^{\dagger} which are linear combinations of electron/hole creation/annihilation operators defined by

$$\begin{aligned} \alpha_{k} &= u_{k}a_{k} - v_{k}b_{-k}^{\dagger}, \qquad \beta_{-k} = u_{k}b_{-k} + v_{k}a_{k}^{\dagger}, \\ \alpha_{k}^{\dagger} &= u_{k}^{*}a_{k}^{\dagger} - v_{k}^{*}b_{-k}, \qquad \beta_{-k}^{\dagger} = u_{k}b_{-k}^{\dagger} + v_{k}^{*}a_{k}. \end{aligned}$$

These operators create/annihilate normalized states with excess quasiparticles orthogonal to $|\Psi\rangle_{BCS}$, which has an equal number of electrons and holes. We can also define the inverse transformations as,

$$\begin{aligned} \alpha_{\mathbf{k}} &= u_{\mathbf{k}}^{*} \alpha_{\mathbf{k}} - v_{\mathbf{k}} \beta_{-\mathbf{k}}^{\dagger}, \qquad b_{-\mathbf{k}} = u_{\mathbf{k}}^{*} \beta_{-\mathbf{k}} + v_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger}, \\ \alpha_{\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} + v_{\mathbf{k}}^{*} \beta_{-\mathbf{k}}, \qquad b_{-\mathbf{k}}^{\dagger} = u_{\mathbf{k}} \beta_{-\mathbf{k}}^{\dagger} + v_{\mathbf{k}}^{*} \alpha_{\mathbf{k}}. \end{aligned}$$

The excited states of BCS theory are states with excess (unpaired) electrons/holes or excited pairs such that

$$|\Psi\rangle = \alpha_{q}^{\dagger} |\Psi\rangle_{BCS} = a_{q}^{\dagger} \prod_{k \neq q} (u_{k} + v_{k} a_{k}^{\dagger} b_{-k}^{\dagger}) |0\rangle.$$
(6.20)

Here, one electron is at q state instead of the ground level. Generalizing this to a variational form we have

$$|\Psi\rangle = \prod_{k} \left(u_{k}^{p} + v_{k}^{+} \alpha_{k}^{\dagger} + v_{k}^{-} \beta_{-k}^{\dagger} \right) \left(u_{k} + v_{k} a_{k}^{\dagger} b_{-k}^{\dagger} \right) |0\rangle$$

$$= \prod_{k} \left(u_{k}^{p} + \left| v_{k}^{+} \alpha_{k}^{\dagger} + v_{k}^{-} \beta_{-k}^{\dagger} \right) \right| \Psi\rangle_{BCS.}$$
(6.21)

The normalization can be achieved by choosing $|u_k|^2 + |v_k|^2 = 1$ and $|u_k^p|^2 + |v_k^+|^2 + |v_k^+|^2 = 1$.

In a thermal state (canonical ensemble) one can write $\langle \alpha_k^{\dagger} \alpha_k \rangle = f(E_k^{\dagger}) = (e^{\beta E_k^{\dagger}} + 1)^{-1}$, where β defines the inverse temperature. Thus,

$$\langle a_{k}^{\dagger}a_{k} \rangle = \left\langle \left(u_{k}a_{k}^{\dagger} + v_{k}^{*}\beta_{-k} \right) \left(u_{k}^{*}\alpha_{k} + v_{k}\beta_{-k}^{\dagger} \right) \right\rangle$$

$$= \left| u_{k} \right|^{2} \left\langle \alpha_{k}^{\dagger}\alpha_{k} \right\rangle + \left| v_{k} \right|^{2} \left\langle \beta_{-k}\beta_{-k}^{\dagger} \right\rangle$$

$$= \left(1 - \left| v_{k} \right|^{2} \right) f_{k}^{+} + \left| v_{k} \right|^{2} \left(1 - f_{k}^{-} \right) = f_{k}^{+} + \left| v_{k} \right|^{2} \left(1 - f_{k}^{+} - f_{k}^{-} \right).$$

$$(6.22)$$

At T = 0, the Fermi function $f_k^{\pm} = 0$, therefore one can recover the usual BCS result as $\langle a_k^{\dagger} a_k \rangle T = 0 = |v_k|^2$. Hence, by applying the properties of canonical transformation, one can write $|u^p v_k|^2 = |v_k|^2 (1 - f_k^{\pm} - f_k^{-}), |v_k^{\pm}|^2 = f_k^{\pm}, |v_k^{\pm}|^2 = f_k^{\pm}$ and $|u^p u_k|^2 = |u_k|^2 (1 - f_k^{\pm} - f_k^{-})$. This signifies the probabilities of having a *pair*, type *a* particle, type *b* particle and *no* particle in the k quantum state. It must be noted here that the formalism is identical with the finite temperature BCS theory where f_k^{\pm} are the occupation numbers of quasi particles.

To derive the mean-field energy gap equation it is now necessary to minimize the Helmholtz free energy with respect to the variational parameters,

$$\left\langle \hat{F} \right\rangle = \left\langle \hat{H} \right\rangle - TS - \mu_a \left\langle \hat{N}_a \right\rangle - \mu_b \left\langle \hat{N}_b \right\rangle,$$

where, $S = -k_B \sum_{k\sigma} \left[f_k^{\sigma} \ln f_k^{\sigma} + (1 - f_k^{\sigma} \ln (1 - f_k^{\sigma})) \right].$ (6.23)

Applying eqs (6.6) and (6.21) one can write,

$$\begin{split} \left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle &= \left\langle \hat{H} \right\rangle = \sum_{k} \left(\varepsilon_{k}^{a} + \varepsilon_{k}^{b} \right) \left| v_{k} \right|^{2} \left(1 - f_{k}^{+} - f_{k}^{-} \right) + \sum_{k} \left(\varepsilon_{k}^{a} f_{k}^{+} + \varepsilon_{k}^{b} f_{k}^{-} \right) \right. \\ &+ \frac{1}{V} \sum_{kk'} U_{q}^{ab} u_{k} v_{k}^{*} u_{k'}^{*} v_{k'} (1 - f_{k}^{+} - f_{k}^{-}) (1 - f_{k'}^{+} - f_{k'}^{-}) \\ &- \frac{1}{2V} \sum_{kk'} U_{q}^{aa} \left| v_{k} \right|^{2} \left| v_{k'} \right|^{2} \left(1 - f_{k}^{+} - f_{k}^{-} \right) (1 - f_{k'}^{+} - f_{k'}^{-}) \\ &- \frac{1}{2V} \sum_{kk'} U_{q}^{bb} \left| v_{k} \right|^{2} \left| v_{k'} \right|^{2} \left(1 - f_{k}^{+} - f_{k}^{-} \right) (1 - f_{k'}^{+} - f_{k'}^{-}) \\ &- \frac{1}{2V} \sum_{kk'} U_{q}^{aa} 2 \left| v_{k} \right|^{2} \left(1 - f_{k}^{+} - f_{k}^{-} \right) f_{k'}^{+} - \frac{1}{2V} \sum_{kk'} U_{q}^{aa} f_{k}^{+} f_{k'}^{+} \\ &- \frac{1}{2V} \sum_{kk'} U_{q}^{bb} 2 \left| v_{k} \right|^{2} \left(1 - f_{k}^{+} - f_{k}^{-} \right) f_{k'}^{+} - \frac{1}{2V} \sum_{kk'} U_{q}^{bb} f_{k}^{-} f_{k'}^{-}. \end{split}$$

If we assume the quasi particle wave functions as, $u_k = \cos \theta_k$ and $v_k = \sin \theta_k$ and rewrite the chemical potential in the following way, $2\xi_k^+ = \xi_k^a + \xi_k^b$,

0

 $2\xi_k^- = \xi_k^a - \xi_k^b$, $2\mu = \mu_a + \mu_b$ and $2h = \mu_a - \mu_b$, then the free energy can be written as,

$$\left\langle \hat{F} \right\rangle = \sum_{k} 2\xi_{k}^{z} \sin^{2} \theta_{k} (1 - f_{k}^{+} - f_{k}^{-}) + \sum_{k} \left(\xi_{k}^{z} f_{k}^{+} + \xi_{k}^{z} f_{k}^{-} \right) + \frac{1}{4V} \sum_{kk'}^{\prime} U_{kk'}^{ab} \sin 2\theta_{k} \sin 2\theta_{k'} (1 - f_{k}^{+} - f_{k}^{-}) (1 - f_{k'}^{+} - f_{k'}^{-}) - \frac{1}{V} \sum_{kk'}^{\prime} U_{kk'}^{aa} \sin^{2} \theta_{k} \sin^{2} \theta_{k'} (1 - f_{k}^{+} - f_{k}^{-}) (1 - f_{k'}^{+} - f_{k'}^{-}) - \frac{1}{V} \sum_{kk'}^{\prime} U_{kk'}^{aa} \sin^{2} \theta_{k} (1 - f_{k}^{+} - f_{k}^{-}) (f_{k'}^{+} + f_{k'}^{-}) - \frac{1}{2V} \sum_{kk'}^{\prime} U_{kk'}^{aa} (f_{k}^{+} f_{k'}^{+} + f_{k}^{-} f_{k'}^{-}) + \frac{1}{\beta} \sum_{k}^{\prime} \left[f_{k}^{+} \ln f_{k}^{+} + (1 - f_{k}^{+} \ln (1 - f_{k}^{+})) \right] + \frac{1}{\beta} \sum_{k}^{\prime} \left[f_{k}^{-} \ln f_{k}^{-} + (1 - f_{k}^{-} \ln (1 - f_{k}^{-})) \right].$$
(6.25)

In the above calculation we have considered that the magnitude of electron–electron and hole–hole interaction is same, that is, $U^{aa} = U^{bb}$. Minimizing eq (6.25) with respect to θ_k and rearranging them we obtain,

$$\tan 2\theta_{k} = \frac{-\frac{1}{2V}\sum_{k'}U_{kk'}^{ab}\sin 2\theta_{k'}(1-f_{k'}^{+}-f_{k'}^{-})}{\xi_{k}^{+}-\frac{1}{2V}\sum_{k'}U_{kk'}^{aa}\left[2\sin^{2}\theta_{k'}(1-f_{k'}^{+}-f_{k'}^{-})+f_{k'}^{+}+f_{k'}^{-}\right]} \equiv \frac{\Delta_{k}}{\xi_{k}}.$$
 (6.26)

Borrowing the analogy from BCS theory we can further write,

$$\sin 2\theta_{k} = \frac{\Delta_{k}}{\sqrt{\xi_{k}^{2} + \Delta_{k}^{2}}} \equiv \frac{\Delta_{k}}{E_{k}}$$

and,
$$\sin^{2} \theta_{k} = \frac{\Delta_{k}^{2}}{2(\Delta_{k}^{2} + \xi_{k}^{2} + \xi_{k}E_{k})} = \frac{1}{2} \left(1 - \frac{\xi_{k}}{E_{k}} \right).$$
 (6.27)

If we now minimize the free energy with respect to f_k^+ and f_k^- , (i.e., $\partial \langle F \rangle / \partial f_k^+ = 0$, $\partial \langle F \rangle / f_k^- = 0$) and carry out necessary rearrangements, we will be able to write the mean-field gap equation. Thus, the coupled equations can be noted as

$$\Delta_{k} = \frac{1}{V} \sum_{k'} U^{ab}_{kk'} \frac{\Delta_{k'}}{2e_{k'}} (1 - f^{+}_{k'} - f^{-}_{k'})$$
(6.28)

$$\xi_{k} = \xi_{k}^{+} - \frac{1}{V} \sum_{k'} U_{kk'}^{aa} \left[\left(1 - \frac{\xi_{k'}}{/} E_{k'} \right) \times \left(1 - f_{k'}^{+} - f_{k'}^{-} \right) + f_{k'}^{+} + f_{k'}^{-} \right]$$

$$E_{k}^{2} = \xi_{k}^{2} + \Delta_{k}^{2}; \quad f_{k}^{\pm} = \begin{cases} 1 & \text{if } E_{k}^{\pm} < 0 \\ 0 & \text{if } E_{k}^{\pm} > 0 \end{cases}$$

$$(6.29)$$

where

$$E_{k}^{\pm} = E_{k} \pm \Delta E_{k}, \ \Delta E_{k} = \Delta \xi_{k} + \frac{1}{2A} \sum_{k'} U_{kk'}^{aa} \left(f_{k'}^{-} - E_{k}^{+} \right), \ \Delta \xi_{k} = \frac{1}{2} \left(\epsilon_{k}^{a} - \mu_{a} - \epsilon_{k}^{b} + \mu_{b} \right).$$

However, the density equations remains unchanged, that is, one needs to follow eqs (6.14) and (6.15).

After solving the coupled equations self-consistently, it is possible to comment on the nature of the bilayer system and their phase separations. Figures 6.5 and 6.6 describe the variation of the energy gap and quasi particle energies with wave vector. However, the interaction energy is chosen differently for both the figures. In Figure 6.5 is calculated only with inter-layer interaction, whereas in Figure 6.6 both intra- and inter-interactions are taken into account. Moreover, in these two figures, the electron and hole numbers are considered as same that is the population balanced case (h = 0) thereby the density imbalance parameter a = 0. Expectedly in the figures we do not observe any variation in occupation number for electrons and holes with varying wave vector. Nevertheless, we can definitely conclude that inclusion of intra-layer interaction suppresses the gap function as evident from the figures.

In the usual mean-field description of the electron-hole bilayer, one uses the bare Coulomb interaction as given in eq (8). In realistic systems, if taken into account the many body effects, it becomes necessary to modify the bare Coulomb interaction. The many body effects can be suitably modeled by a screening function which usually decreases the strength of the bare Coulomb interaction for electrons and holes in the normal phase. However, it is difficult to model an exact 2D screening function due to intra- and inter-layer interactions for condensed phase. Nevertheless for a qualitative understanding, one can consider the mechanism of

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FIGURE 6.5 The left side figure depicts variation of Gap function, quasi-particle energies with wave vector for balanced density ($\alpha = 0$) and $r_s = 3$. The right side figure describes the variation of occupation number with wave vector. In this calculation, only interlayer interaction is taken into account.⁵⁸



FIGURE 6.6 Both the figures are similar with Figure 6.5 in parameter values and observables; however in this figure, both inter-layer and intra-layer interactions are taken into account.⁵⁸

gate screening. In this mechanism, the Coulomb potential of a point charge is replaced by that of a dipole consisting of the point charge and its image behind the metallic gate. An approximate description of the screening by the gate potential after taking into account the intra- and inter-layer interactions can be expressed as,⁴⁹

$$U_{q}^{aa} = U_{q}^{bb} = \frac{2\pi e^{2}}{\varepsilon \sqrt{q^{2} + \hat{e}^{2}}}, \qquad U_{q}^{ab} = \frac{2\pi e^{2}}{\varepsilon \sqrt{q^{2} + \hat{e}^{2}}} e^{-qd}, \qquad (6.30)$$

respectively, where the parameter κ is a screening wave number. In the calculation, the screening length associated with gate screening is considered as ~ $20a_{R}$, that is, $\kappa = 1/20a_{R}$.

In Figures 6.7 and 6.8, the variation of gap function, quasi particle energy, and occupation number with wave vector is depicted for bare Coulomb interaction. In the numerical calculations, GaAs system parameters are taken into account where mass ratio turns out to be $m_d/m_b = 0.07/0.30$ and background dielectric constant is $\varepsilon = 12.9$.



FIGURE 6.7 Gap function and quasi-particle energies associated with Sarma-2 phase at $r_s = 3$ and $\alpha = -0.3$ (excess hole) is depicted with bare Coulomb interactions for $m_e m_h = 0.07/0.30$ and $d = a_B^{.59}$

The solutions of energy gap, quasi particle energies, and occupation numbers are illustrated in Figures 6.7 and 6.8 for bare Coulomb interaction. The screened Coulomb counter part is presented in Figures 6.9 and 6.10. In all the cases the inter-layer distance is considered as one Bohr radius ($d = a_B$). The figures show the gap function (Δ_k), the quasi-particle energies (E_k^+) and their average (E_k) on the left panels, and the electron and hole occupation numbers $n_a(k)$, $n_b(k)$ on the right panels. At T = 0 in the ground state, the quasi-particle levels with negative energy are occupied, positive energy levels are empty. The two different type of excitation branches can be observed due different electron-hole mass and chemical potential values. When one of the spectra crosses the zero energy axis, population imbalance is created. If the negative energy region includes the origin at k = 0, the ground state has one Fermi surface defined as S1 (as evident in Figs. 6.8 and 6.10), otherwise it has two S2. Since the quasi-particle energy branch is continuous, the system still has gapless excitations. A close investigation of the gap function Δ_k in the absence of screening (Figs. 6.7 and 6.8) shows that it has a cusp at the zero crossings of the quasi-particle energy, corresponding to a divergence in the derivative of Δ_k . This divergence leads to important consequences on the stability of the Sarma phase at T = 0.



FIGURE 6.8 Gap function and quasi-particle energies associated with Sarma-1 phase at $r_s = 5$ and $\alpha = 0.5$ (excess electron) is depicted with bare Coulomb interactions for $m_e/m_h = 0.07/0.30$ and $d = a_{B^*}^{.59}$



FIGURE 6.9 Gap function and quasi-particle energies associated with a Sarma-2 phase at $r_s = 2.5$ and $\alpha = 0.2$ (excess electrons) in presence of screened Coulomb interactions for $m_e/m_h = 0.07/0.30$ and $d = a_B$ is illustrated. The lower panel show a Sarma-1 phase at $r_s = 5$ and $\alpha = 0.5$ with excess electrons. Occupation numbers are shown on the right.⁵⁹



FIGURE 6.10 Gap function and quasi-particle energies associated with a Sarma-1 phase at $r_s = 5$ and $\alpha = 0.5$ (excess electrons) in presence of screened Coulomb interactions for $m_e/m_h = 0.07/0.30$ and $d = a_B$ is described.⁵⁹

After elaborating the presence of Sarma phases it is now important to explicate their stability issue. The stability is usually understood by calculating the superfluid mass density.⁴⁸ This quantity should be positive in a stable state and a negative value is identified with an instability towards an FFLO phase.⁴⁸ The positivity of the superfluid mass density ensures that the Sarma phase is a local minimum of the energy with respect to fluctuations of the gap parameter. However, there exists another possibility of an FFLO phase with finite pair momentum leading to a global minimum of the energy. When this happens, the local stability of the Sarma phase is known as metastability.

The superfluid mass density is given by⁴⁹

$$\boldsymbol{\rho}_{s} = m_{e}n_{e} + m_{h}n_{h} - \frac{\hbar^{2}\beta}{8\pi}\int dkk^{3} \frac{1}{2} \left[\frac{1}{\cosh^{2}(\beta E_{k}^{+}/2)} + \frac{1}{\cosh^{2}(\beta E_{k}^{-}/2)} \right]$$
(6.31)

where β is the inverse temperature. At T = 0 this expression can be written as⁴⁸

$$\operatorname{For} \rho_{s} = m_{e}n_{e} + m_{h}n_{h} + \frac{\hbar^{2}}{4\pi} \sum_{j,\lambda} \frac{\left(k_{j}^{\lambda}\right)^{3}}{\left|\frac{dE_{k}^{\lambda}}{dk}\right|_{k=k_{j}^{\lambda}}} \qquad (6.32)$$

where k_j^{λ} are the roots of E_k^{λ} with $\lambda = \pm$. At zero temperature the last expression involves the derivative of Δ_k at the zero crossings of E_k^{\pm} . However, it has been observed that numerical analysis turns our more efficient if the calculation is carried out for $T \rightarrow 0$ instead of T = 0. The numerical simulation reveals that the derivative of the gap energy diverges logarithmically as $T \rightarrow 0$. An analytical calculation demonstrates that for the bare Coulomb interaction as

$$\frac{\mathrm{d}\Delta_{k}}{\mathrm{d}k}\Big|_{k=k^{*}} \approx \frac{e^{2}}{\pi\varepsilon 2E_{k^{*}}} |\ln T| \quad \text{as} \ T \to 0$$
(6.33)

where k^* is the zero crossing point at T = 0 as $k \to k^*$

$$\frac{\mathrm{d}\Delta_{k}}{\mathrm{d}k}\Big|_{T=0} \approx \frac{e^{2} \Delta_{k^{*}}}{\pi \varepsilon 2E_{k^{*}}} \ln \left|k-k^{*}\right| \quad \text{as} \ k \to k^{*}, \tag{6.34}$$

This divergence is due to the presence of the long-range Coulomb interaction, which is singular at q = 0, and due to the discontinuity of the Fermi function at T = 0. Since at finite temperature, the discontinuity of the Fermi function is smeared out, the divergence is also removed. Same argument can be applied for screening potential in place of bare Coulomb interaction.

The phase diagram presented in Figure 6.11 originates from the comparison of the energies of the Sarma and normal phases and their stability scenario. As usual in the calculation, the inter-layer separation is taken as $d = a_{B}$. Figure 6.11 can be considered as a continuation of the phase diagram presented in Figure 6.4, where the diagram was continuously modified to take into account different realistic situations. In precise, the top-left figure is drawn for bare inter-layer interactions only; in the adjacent figure, intralayer interaction is also added. The bottom-left figure depicts the phases for screened inter-layer interactions only, whereas the bottom right one is generated for screened inter- and intra-layer interactions.

For bare interactions, the superfluid density is always positive and the Sarma phase is stable locally as discussed earlier. Hence the top-left figure does not include the FFLO phase. However as mentioned earlier, there remains the possibility of first-order transition to FFLO phase. Therefore in the top panel two topologically distinct Sarma phases, Sarma-1 with one Fermi surface and Sarma-2 with two Fermi surfaces can be seen. The intra-layer repulsive interactions will try to delocalize the charge carriers which effectively favor the normal phase with respect to the condensed phases.

This phenomenon can be seen in the top-right figure as the r_s required to increase to draw the phase boundary between normal and condensed phases.

The bottom panel of Figure 6.11 presents the phase diagram when the gate screening is taken into account. In presence of the screening, interlayer interactions itself induces Sarma phases to be unstable for a large portion of the phase diagram, especially with excess holes, that is, $\alpha < 0$ and one can only find S1 phase making S2 phase completely absent. However, switching on the intra-layer interactions reduces the space occupied by the FFLO phase and S2 phase can be obtained for small region in the phase diagram. Usually, the FFLO modulations of the gap function is accompanied by some density modulation in the real space. The repulsive Coulomb interaction does not favor such density modulations as an effect one cannot find FFLO states in presence of bare Coulomb interaction thereby ensuring a dominant Sarma phase. Therefore, the phase diagram becomes more intriguing when both intra-layer and screening effects are present. The presence of locally stable Sarma phases confirms that gapless superfluid states can be stable with momentum dependent interaction.



FIGURE 6.11 Zero temperature phase diagram for d = 1. The dashed line indicates $\mu = 0$ and the dashed dotted line indicates the separation between S1 and S2 phases.⁵⁹

6.2.1.4 COMMENTS ON INCLUSION OF IMPURITY

From the above discussion, it is very clear that the interplay of interactions enriches the phase diagram dramatically and certain new phases emerge. We expect this situation will become more novel if we include some disorder. Here, we present a brief idea of how the disorder can be included in the mean-field formalism. It is in the same spirit as the usual atomic BCS–BEC crossover.

In atomic BCS–BEC crossover, a small amount of impurity can be embedded in the system by means Gaussian fluctuations. For that purpose, we will use the path integral formalism where we consider the Nambu propagator as

$$G^{-} = G_0^{-1} - V_d(q)\sigma_z, (6)$$

where $V_d(q)$ is the disorder potential. We define,

$$G_{0}^{-1} = \begin{pmatrix} i\omega + \xi_{k}^{b} & \Delta_{k}^{0} \\ \overline{\Delta}_{k}^{0} & i\omega - \xi_{k}^{b} \end{pmatrix}.$$
(6.36)

We also assume small fluctuation about the pairing gap, that is, $\Delta_k = \Delta_k^0 + \delta \Delta_k$, where Δ_k^0 is the pairing gap in the clean system and it causes small fluctuation $\delta \Delta_k$ in presence of disorder. Hence the self-energy can be written as,

$$\sum = -V_d(q)\sigma_z + \delta\Delta_k(q)\sigma^+ + \delta\overline{\Delta}_k(-q)\sigma^-.$$
(6.37)

From eq (6.11), one needs to calculate the effective action appropriately. For that purpose we can rewrite $\ln (1 + \Sigma G_0) = G_0 \Sigma - \frac{1}{2} (G_0 \Sigma' G'_0 \Sigma)$ when the Dyson equation is expanded till the second order. Hence the path integral over $\frac{\Delta \overline{\Delta}}{U}$ – Tr ln G^{-1} can be expressed as sum of Bosonic action (S_B) , fermionic action (S_F) and the action related to saddle point calculation S_0 . In other terms, S_0 is the first order in the Dyson equation and for any extremum in the total action this term must be equated to zero. Therefore the effective action can be written as $S_{eff} = S_B + S_0 + S_F$. A detailed calculation reveals

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$$S_{B} = \sum_{k} \left[\frac{\Delta_{k}^{0}}{U_{kk'}} + \sum_{k'} \frac{\Delta_{k'}^{0}}{2E_{k'}} (1 - f_{k'}^{+} - f_{k'}^{+}) \right] \left[\delta \Delta_{k}(0) + \delta \overline{\Delta}_{k}(0) \right]. \quad (6.38)$$

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Applying the saddle point condition $\left(\frac{\delta S_{eff}}{\delta \Delta} = 0\right)$, one can write

$$\Delta_{k}^{0} = -\frac{1}{V} \sum_{k'} U_{kk'} \frac{\Delta_{k'}^{0}}{2E_{k'}} \left(1 - f_{k'}^{+} - f_{k'}^{+} \right)$$
(6.39)

The fermionic action can be expressed as

$$S_{F} = \beta \sum_{kk'} \frac{\Delta_{k}^{0} \overline{\Delta}_{k}^{0}}{U_{kk'}} - \frac{1}{\beta} \sum_{k,i\omega} \left[Tr \ln\left(-G_{0}^{-1}(k)\right) + V_{d}(0)\sigma_{z}\right) \right] + \Omega_{Fd},$$

where, $\Omega_{Fd} = \frac{1}{2\beta} \sum_{k,q} \operatorname{Tr}\left[G_{0}(k)\sigma_{z}G_{0}(k+q)\sigma_{z}\left\langle V_{d}(q)V_{d}(-q)\right\rangle\right].$
(6.40)

The bosonic action arising through fluctuation and impurity can be written as

$$S_{B} = \frac{1}{2} \sum_{q} \left[V_{d}(q) \chi \lambda^{\dagger} + V(-q) \chi^{\dagger} \lambda + \lambda^{\dagger} M \gamma \right], \tag{6.41}$$

where

$$\chi = \begin{pmatrix} A_{k+q} \Gamma_k - B_k \Gamma_{k+q} \\ A_k \overline{\Gamma}_{k+q} - B_{k+q} \overline{\Gamma}_k \end{pmatrix}, \qquad \lambda = \begin{pmatrix} \delta \Delta_k(q) \\ \delta \overline{\Delta}(-q) \end{pmatrix}$$

Here for the convenience of calculation, we have redefined the Greens functions in the following way

$$G_0(k) = \begin{pmatrix} A_k & \Gamma_k \\ \overline{\Gamma}_k & B_k \end{pmatrix}, \quad G_0(k+q) = \begin{pmatrix} A_{k+q} & \Gamma_{k+q} \\ \overline{\Gamma}_{k+q} & B_{k+q} \end{pmatrix}.$$
 (6.42)

However, one can always look back to eq (6.36) for exact form of the Green's function. The last term in the bosonic action turns out as

$$\lambda^{\dagger} M \lambda = \left(\delta \overline{\Delta}_{k}(-q), \delta \Delta_{k}(q) \right) \begin{pmatrix} \frac{1}{U_{kk'}} + A_{k+q} B_{k} & \Gamma_{k} \Gamma_{k+q} \\ \overline{\Gamma}_{k} \overline{\Gamma}_{k+q} & A_{k} B_{k+q} \end{pmatrix} \begin{pmatrix} \delta \Delta_{k}(q) \\ \delta \overline{\Delta}(-q) \end{pmatrix}$$

It is well known that that $\frac{1}{\beta} \frac{\partial S_F}{\partial \mu_i} = n_i$ for the clean Fermi system. However, if we consider the existence of fluctuation and insert the impurity we obtain non zero bosonic action. Hence for system described above, one needs to apply

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$$\frac{1}{\beta} \frac{\partial S_{eff}}{\partial \mu_i} = n_i$$

$$\frac{1}{\beta} \left[\frac{\partial S_F}{\partial \mu_i} + \frac{\partial S_B}{\partial \mu_i} \right] = n_i$$
(6.43)

Using the modified density equation along with the gap equation, one can now examine the effect of impurity in the phase separation of a bilayer system in a semiconductor.

6.2.2 EXPERIMENTS WITH EXCITONS

In the above discussion, we have elaborated the consequence of interplay of different types of interaction by means of mean-field theory. This we explicate with analogy from the atomic BCS-BEC crossover. However, it is interesting to note that excitons were first to be considered for the BCS-BEC crossover.⁶¹ On the reverse path, experiments with population imbalance in ultra-cold trapped Fermi atoms⁶⁰ have stimulated a considerable amount of theoretical work on two-component Fermi systems with density imbalance.^{62,63} This upsurge in interest actually derives from the expectation of exotic phases in addition to the ordinary BCS pairing.^{62,64,65} However, the presence of a trap and charge neutrality of the atoms inhibit the occurrence of many of the exotic phases. Therefore excitons are considered as a good candidate for observing such exotic phases because the Coulomb repulsion within each layer acts to suppress phase separation.⁶⁶ Additionally, it is worth noting that the different electron and hole effective masses in GaAs, $m_{\rm e}$ and $m_{\rm h}$, and the non-local nature of the electron-hole attraction both favor the occurrence of exotic phases.48

In recent years, using electrical and optical techniques exciton condensation has been observed in several different systems. Quantum Hall experiments at half-filling investigate BEC in electron–electron and hole– hole bilayers. Optically generated bilayer excitons also show evidence for condensation. Off-late, excitons coupled to photons to form polaritons with even smaller mass leading to higher condensation temperatures have been experimentally detected.⁵⁸ In the last couple of years, scientist are even able to form a droplet (about five electron–hole pairs together inside semiconductor) made up of electron–hole bilayers systems.⁶⁷ This is popularly known as dropleton. The creation of dropletons was carried out in an electron-hole plasma inside a *GaAs* quantum well by ultrashort laser pulses. As the name suggested dropleton are the first quasiparticle found to behave like a liquid. This discovery was sudden and the scientist had no idea about such property a priori. This emphasizes the richness of the context of bilayer systems. Also, it reminds that there are many issues to unravel in the process to understand this system properly.

6.3 APPLICATIONS

The importance of excitonic research lies in its multifacet possible applicability. The current interests of different scientific and engineering endeavors are mostly getting converged to the field of energy and communication. Already there are different techniques of solar cells and microchips which have made substantial enrichments in these fields but it is still far beyond the goal. In the domain of information technology and computation, the idea of quantum computers and simulators are already been placed. From a theoretical point of view, quantum information processing can be considered as a well-established field by now but the key issue of the design and realization of concrete solid-state implementation protocols are subject of intense investigation at the moment.

Recently, several proposals are placed for an all optical implementation of quantum information/computation with semiconductor macroatoms (quantum dots in zero dimension). These quantum dots can be defined as a portion of matter (say semiconductor) whose excitons are confined in all three spatial dimensions. The quantum hardware consists of an array of quantum dots and the computational degrees of freedom are energyselected inter-band optical transitions. The quantum-computing strategy exploits exciton-exciton interactions driven by ultrafast multicolor laser pulses. It allows a subpicosecond, decoherence-free, operation time scale in realistic semiconductor nanostructures.^{68,69} Also, there exist proposals based on charge-plus-spin degrees of freedom in semiconductor quantum dots.⁷⁰ These propositions encourage a coherent optical control of electronic spins as well as of excitonic state. In addition, a proper tailoring of exciton-exciton Coulomb coupling (allowing for the implementation of single- as well as two-qubit gates) can introduce the full set of basic operations to implement quantum computing.

Through the above discussion, we have tried to highlight the intriguing technological issues which are mainly governed by the physics of electron–hole systems. Therefore in this chapter, we have tried to narrate a theoretical perspective to present an overview for the electron–hole bilayer systems in semiconductors.

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KEYWORDS

- semiconductor
 - electron-hole system
 - Bose-Einstein condensate
- resonance stabilization
- intra-layer interaction

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