Mean-Field Theory for the Spin-Triplet Exciton Liquid in Quantum Wells

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Using a mean-field theory, we study the possible existence of a spin-triplet intersubband exciton liquid ground state in semiconductor quantum well systems as a function of the electronic density and the strength of the intersubband Coulomb interaction matrix element at low temperatures. We find the excitonic phase to be stable over a large region of parameter space, and our calculated critical temperatures are attainable experimentally. In addition, we find that the transition to the excitonic phase can be either first- or second-order at zero temperature.

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FIG. 1. Change in the electronic dispersion from the normal phase with two subbands occupied (left side of the figure) to the excitonic phase (right side of the figure). In the normal phase, the band structure consists of two subbands (0 and 1), each with degenerate spin-up (+) and spin-down (-) components; in the excitonic phase, the band structure still contains two subbands, but they are linear combinations of the original bands that result in a larger subband splitting and the occupation of only the lowest subband. In both cases, all states below the chemical potential $\mu$ are filled at zero temperature.

Interest in the effects of electronic correlations in low-dimensional quantum systems such as quantum wells and quantum wires is motivated by both applied and basic science objectives. On the applications side, the continuing reduction in the characteristic size of the components of integrated circuits suggest that quantum effects will eventually become important design considerations in these devices. In addition, the unusual electronic properties of low-dimensional quantum systems present the possibility of developing new devices to exploit these properties. On the basic science side, low-dimensional quantum systems are almost ideal realizations of simple quantum mechanical systems, and so are test-beds for our understanding of single- and many-particle aspects of quantum mechanics. In particular, the ability to enter a regime where electronic correlation effects become large opens the possibility of discovering new, strongly correlated quantum phases, as has already happened with the fractional quantum Hall effect. In this paper, we describe another possible correlation-driven phase which occurs in low-dimensional quantum systems in the absence of a magnetic field: the spin-triplet exciton liquid.

The existence of this phase was recently predicted theoretically by Das Sarma and Tamborenea based on a local-density approximation (LDA) calculation of the collective mode spectra of either double or wide single quantum wells. In these calculations, the frequency of the long-wavelength intersubband spin-density excitations vanishes for electron densities around $10^{10}$ to $10^{11}$ cm$^{-2}$. This mode softening implies that intersubband spin-density excitations are spontaneously generated in the system and thus signals the presence of a new phase. However, bulk semiconductors possess a three-dimensional structure and a (usually indirect) energy gap between the conduction and valence bands. By contrast, we consider here the conduction subbands in modulation-doped two-dimensional semiconductor microstructures which do not have a gap in their (two-dimensional) single-particle excitation spectra [cf. the left side of Fig. 1]. Thus, in order to describe the phase predicted by Das Sarma and Tamborenea, it is necessary to reconsider the theory of the exciton liquid within the context of quantum wells.

As yet, no definitive experimental evidence for the existence of the excitonic phase has been presented; indeed, beyond the softening of the intersubband spin-density excitations, no calculations exist about the properties of the new phase. However, the collective mode softening should be observable by inelastic light scattering techniques. Moreover, the use of the LDA to compute the collective modes in quantum wells in both the charge
and spin channels is well established and yields good agreement with experiment, even when many-body effects become important. We therefore expect that the excitonic phase should be observed experimentally in the future. In anticipation of this discovery, we present here a brief description of the spin-triplet exciton phase based on a mean-field theory. We determine the nature of the new phase and establish its boundaries in temperature, density, and intersubband Coulomb repulsion. A more detailed description of these calculations, along with a computation of the collective modes and the effect of impurities on the excitonic phase, will appear elsewhere. 

The physical system we wish to describe consists of an electron gas in the presence of a confining potential along the $z$-direction which interacts via a screened Coulomb repulsion. The confining potential may be viewed as arising from either a double quantum well or a wide single quantum well; in either case, the two lowest-energy bound states of the confining potential are well separated in energy from the next-lowest energy level. This situation can arise, for example, in the lowest symmetric-antisymmetric subband splitting in a double quantum well structure. Since we wish to focus on the general features of the condensed phase and not on the detailed effects arising from the wave-vector and frequency dependence of the screened Coulomb interaction, we take the interaction to be a short-range repulsion. In principle, we may include more detailed forms of the interaction within our mean-field formalism, but these detailed calculations should not affect the qualitative features we will discuss. Furthermore, the short-range repulsion model has the advantage of being a single-parameter description of the interaction and should be a reasonable approximation at densities which are not too low.

We work in the basis defined by the product of eigenstates of the confining potential $\xi_\alpha(z)$ and two-dimensional free particles $e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V_0}$. In this basis, the Hamiltonian may be written

$$H = \sum_{\alpha k \sigma} \left[ E_\alpha - \frac{\hbar^2 k^2}{2m} - \mu \right] c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} + \frac{1}{2V_0} \sum_{\alpha k_1, q \sigma_1, \alpha k_2, q_2} V_{\alpha_1 \alpha_2 \alpha_3} c_{\alpha_1 k_1 + q_1 \sigma_1}^\dagger c_{\alpha_2 k_2 - q_2 \sigma_2} c_{\alpha_3 k_2 \sigma_2} c_{\alpha_1 k_1 \sigma_1},$$

where

$$V_{\alpha_1 \alpha_2 \alpha_3} = \int dz \xi_{\alpha_1}^*(z) \xi_{\alpha_2}^*(z) \xi_{\alpha_3}(z) \xi_{\alpha_4}(z)$$

(1)

is the matrix element of the short-range interaction $V$, $V_0$ is the area (2D volume) of the confined electron gas, $\mu$ is the chemical potential, $E_\alpha$ is the subband eigenenergy of the bound state $\alpha$ of the confining potential, and $c_{\alpha k \sigma}$ annihilates an electron of effective mass $m$ in subband $\alpha$ with wave vector $k$ and spin projection $\sigma$.

To make the calculations more tractable, we take advantage of several symmetries in the problem and make some simplifying approximations. First, the two lowest subbands are by assumption well separated from the others, so we consider only these subbands, as depicted by the left diagram in Fig. (1). This should be an excellent approximation for energies and temperatures much less than the splitting between the lowest and third lowest subbands. Second, we may take the wave functions $\xi_\alpha(z)$ to be real, so that the ordering of the indices in the Coulomb matrix elements is irrelevant. Third, we make the reasonable assumption that the confining potential is even in $z$, so that $V_{01,11} = V_{10,00} = 0$ ($\alpha = 0$ (1) denotes the (next to) lowest subband). The remaining independent matrix elements are then $V_{00,00}$, $V_{01,11}$, and $V_{00,11} = V_{10,10}$. Finally, for the problem in which we are interested, we may set $V_{00,00} = V_{11,11} = 0$ without loss of generality. These diagonal matrix elements act to renormalize the subband splittings and give rise to ferromagnetic phases at low densities. While our formalism can easily incorporate these matrix elements, we are primarily interested in the excitonic phase, so we leave the detailed effect of these matrix elements as a subject for future work. 

We solve this two-subband model within mean-field theory. The propagators and self-energies are defined in the usual way as matrices in the subband index and spin projection. With these quantities, we set up and solve the one-loop self-consistent Hartree-Fock equations depicted by the diagrams of Fig. (2(a)). We simultaneously impose the constraint that the chemical potential yield a fixed electronic density $n$. In evaluating the mean-field theory, we allow for the possibility of self-energies which are off-diagonal in both spin and band indices. Since the LDA calculations of Das Sarma and Tamborenea indicate that the intersubband spin-density excitations soften in the excitonic phase we expect that thermal averages of the form $\Delta_{\alpha \sigma} = \langle c_{\alpha \sigma}^\dagger c_{\alpha \sigma} \rangle - \langle c_{\alpha \sigma}^\dagger \rangle \langle c_{\alpha \sigma} \rangle$ will become non-zero in the excitonic phase. In the language of critical phenomena, $\Delta_{\alpha \sigma}$ is the order parameter of the phase transition, and $\Delta_{\alpha \sigma} \neq 0$ indicates the spontaneous breaking of the intersubband spin symmetry which leads to the excitonic phase.

Indeed, the resulting mean-field equations have two classes of solutions: a paramagnetic phase where $\Delta_{\alpha \sigma} = 0$ with either one or both subbands occupied, and an excitonic phase where $\Delta_{\alpha \sigma} \neq 0$. Direct calculation of the order parameter in the excitonic phase shows that it is independent of $\alpha$ and $\sigma$ and may be written as $\Delta = \sqrt{(nV_{01}/2)^2 - \Delta_{\text{SAS}}^2}$, where $\Delta_{\text{SAS}} = E_1 - E_0$ is the splitting between the lowest two subbands. Taking the expectation value of the Hamiltonian [Eq. (1)] in the interacting ground state and evaluating it within the mean-field approximation [Cf. Fig. (2(b))], we find that the excitonic phase is stable when $2n_0V_{01} \geq 1$ and $nV_{01} \geq 2\Delta_{\text{SAS}}$. (In this expression, $N_0 = m/2\pi\hbar^2$ is the two-dimensional, single-spin density of states). We also find that, despite the spin-triplet nature of the order parameter, there is no net magnetic moment in the excitonic phase, similar
to what happens in the Balian-Werthammer description of the B-phase of superfluid $^3$He.[21]

Examining the excitation spectrum of the excitonic ground state shows that it is characterized by a rearrangement of the non-interacting bands, as shown in Fig. 1. The interacting bands become linear combinations of, for example, the spin-up portion of subband 0 and the spin-down portion of subband 1. These combinations are expected from the form of the order parameter $\Delta_{\alpha\sigma}$ and may also be obtained from a Bogoliubov transformation of the original Hamiltonian. The new combinations increase the effective splitting between the subbands and so reduce the potential energy associated with the intersubband Coulomb repulsion. Moreover, if the second subband is occupied in the normal phase, the de-population of the second subband in the excitonic phase reduces the kinetic energy of the system. These two effects stabilize the excitonic phase when the intersubband Coulomb interaction is sufficiently large. We note that the interacting single-particle density of states is not gapped in the excitonic phase, so the new ground state is neither an insulator nor a BCS-like superconductor. Thus, the phase transition to the spin-triplet exciton liquid may be difficult to observe in transport measurements.

At zero temperature, these results may be summarized in the phase diagram of Fig. 3. There are three regions of interest in this figure: $N_1$, corresponding to the normal phase with only one subband occupied; $N_2$, corresponding to the normal phase with both subbands occupied; and the excitonic phase. As may be seen from the expression for the order parameter, the phase transition from $N_1$ to the excitonic phase is second-order (solid line), but the transition from $N_2$ is first-order (dashed line). In the figure, $N_0 = m/2\pi\hbar^2$ is the single-spin, 2D density of states, and $\Delta_{\mathrm{SAS}} = E_1 - E_0$ is the splitting of the lowest two subbands in the normal phase.

We have also examined the finite-temperature properties of the mean-field theory and find that the excitonic phase is stable up to a finite temperature $T_c$ which can be several times $\Delta_{\mathrm{SAS}}/k_B$. This critical temperature is plotted as a function of the electronic density $n$ and the intersubband repulsion $V_{01}$ in Fig. 4. Since $\Delta_{\mathrm{SAS}}/k_B$ can be on the order of 10 K or more, the excitonic phase should be experimentally observable. We note that our calculation of $T_c$ includes all components of the self-energy and so is analogous to the strong-coupling theory of superconductivity.[22] Consequently, our calculated $T_c$ is the best estimate of the actual critical temperature available within mean-field theory. However, since mean-field theories are known to overestimate critical temperatures in two-dimensional systems, we cannot rule out the possibility of having very low transition temperatures in real systems.

We have treated $V_{01}$ and $n$ independently in this calculation, but in actual systems $V_{01}$ is determined by $n$ and the geometry of the quantum wells. To make a quantitative comparison of our theory with experiment therefore requires a detailed calculation of the intersubband Coulomb matrix element $V_{01}$. This computation may be accomplished with an LDA theory (see, for example,
the normal-state splitting of the lowest two subbands. Since $\Delta_{\text{SAS}} = E_1 - E_0$ is the single-spin, 2D density of states, and $\Delta_{\text{SAS}} = E_1 - E_0$ is the normal-state splitting of the lowest two subbands. Since $\Delta_{\text{SAS}}/k_B$ is usually on the order of 10 K or more, the excitonic phase may be experimentally observable in suitably constructed quantum wells.

Ref. 6 and will result in a particular path within the parameter space of the phase diagram of Fig. 3. Whether the excitonic phase is observable for that geometry then becomes a question of detail; specifically, does the resulting trajectory pass into the excitonic regime? The calculations of Ref. 6 suggest that many quantum well systems can enter the excitonic phase for low but obtainable electronic densities, so our calculations should be relevant to these systems.

To summarize, we have developed a mean-field theory which describes a new phase in two-dimensional quantum systems, namely the spin-triplet intersubband exciton liquid. This phase should appear in double or wide single quantum wells when the intersubband Coulomb interaction is large, the intersubband energy separation is small, the electronic density is low, and at temperatures which may be accessible experimentally. We have constructed the mean-field phase diagram for the excitonic phase assuming that the intersubband repulsion and the electronic density may be varied independently, and we find regions of both first- and second-order phase transitions at zero temperature. Further experimental and theoretical work is required in order to observe and quantify more precisely the properties of this phase and its relationship to other phases of low-dimensional systems such as Wigner crystals and ferromagnets.

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