PHASE DIAGRAM AND SKYRMION ENERGY FOR BILAYER HETEROSTRUCTURES AT INTEGER FILLING FACTORS

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Phase diagram of a bilayer heterostructure at integer filling factors was established using the hidden symmetry method. Three phases: ferromagnetic, canted antiferromagnetic (CAP) and spin-singlet, have been found. We confirm early results of Das.Sarma et al. Each phase violates the SU(4) hidden symmetry and is stabilized by anisotropy interactions. A charged excitation in bilayer: skyrmion, has been found and its anisotropic energy gap has been calculated. The gap has a prominent minimum in the CAP.

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Integer filling factors ν of Landau Level in hetero-structure 2D electron gas (2DEG) are of special interest. Here the ground state is non-degenerate and the Hartree – Fock approximation (HFA) can be applied with the accuracy limited only by a small ratio of the Coulomb interaction energy to the energy of cyclotron resonance. The ground state of a single layer at $\nu=1$ is a ferromagnet with the elementary excitations being spin excitons or spin-waves. These are gapless [1] in the exchange approximation and do not interact with each other for vanishing momenta [2]. Both are consequences of the exact symmetry under spin rotation. In Ref.[3] a special spin texture in 2DEG ferromagnet: skyrmion [4], was predicted as an elementary charged excitation. The energy of neutral skyrmion-antiskyrmion pair is just a half of the spin exciton energy.

In a bilayer 2DEG the HFA applies only in two cases. The first one corresponds to well separated layers which is a common setup in the experiment [5, 6]. Here one starts from the two single layer ferromagnets and makes a perturbation expansion in powers of interlayer interactions [7]. The second one is the symmetric case where the bilayer Hamiltonian is invariant under SU(4) rotations in both layer and spin spaces. Here all symmetry breaking fields like Zeeman must be negligible. The first attempt in this direction dealt with the case $\nu = 1$ and spin polarized electrons [8, 9]. Recent works [10, 11] that specialize to the bilayer case $\nu = 2$ employ the HFA and predict three distinct phases: ferromagnetic, CAP and a spin-singlet phase. Our approach is similar to that of Refs.[11] but we show explicitly that the HFA is exact in the SU(4)symmetric bilayer. Anisotropy terms reduce the symmetry to $SU(2) \otimes SU(2)$ and lift the eigen state degeneracy. But there are no Fermi-liquid type renormalizations of the anisotropy Hamiltonian due to the symmetric Hamiltonian. We prove the stability of all phases with respect to long-range spatial perturbations. Our work was motivated by recent measurement of the diagonal conductivity activation energy in bilayer [6], which we identify with the energy gap of topological excitation: skyrmion, in an SU(4) Sigma Model. Calculated in this letter skyrmion's energy gap has a profound minimum in the CAP, in line with the findings of Ref. [6].

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The Hamiltonain of a 2DEG in a confining potential $V(\rho)$ and in an external magnetic field H reads:

$$H = \int \psi_{\alpha}^{+}(\boldsymbol{\rho}) \left(\frac{1}{2m} \left[-i \nabla + \boldsymbol{A}(\boldsymbol{\rho}) \right]^{2} + V(\boldsymbol{\rho}) - |g| \mu_{B} H \sigma_{\alpha\beta}^{z} \right) \psi_{\beta}(\boldsymbol{\rho}) d^{3} \boldsymbol{\rho} + \frac{1}{2} \int \int \frac{e^{2}}{\kappa |\boldsymbol{\rho} - \boldsymbol{\rho}'|} \psi_{\alpha}^{+}(\boldsymbol{\rho}) \psi_{\beta}^{+}(\boldsymbol{\rho}') \psi_{\beta}(\boldsymbol{\rho}') \psi_{\alpha}(\boldsymbol{\rho}) d^{3} \boldsymbol{\rho} d^{3} \boldsymbol{\rho}',$$

$$(1)$$

where κ is the dielectric constant, $\alpha, \beta = \pm$ are spin indices and thereafter a sum over repeated indices is implied. We use units: $\hbar = 1$, e = c and H = B = 1 and distances are expressed in terms of the magnetic length: $l_H = \sqrt{c\hbar/eH} = 1$. We split ρ into a coordinate ξ perpendicular to the layer and two in-plane coordinates $\mathbf{r} = (z, \bar{z})$ and assume the confining potential to be uniform over the plane: $V(\rho) = V(\xi)$, with the two wells being separated by a distance d. Two eigen functions: the lowest energy symmetric and the lowest energy antisymmetric can be rotated into $\chi_{1,2}(\xi)$ eigen functions localized in one layer. We expand an electron operator in terms of these two eigen functions: $\psi_{\alpha}(\rho) = \chi_{\tau}(\xi)\phi_{p}(\mathbf{r})c_{\alpha\tau p}$, where $c_{\alpha\tau p}^{+}$ and $c_{\alpha\tau p}$ are electron creation and anhilation operators, $\phi_{p}(z\bar{z})$ is the lowest LL wave function number p, the index $\tau = 1, 2$ being the layer index. We assume the case of a sufficiently strong magnetic field with the cyclotron energy 1/m dominating over the Coulomb, Zeeman and the level splitting: $t = E_A - E_S$, energies.

The Coulomb interaction matrix can be projected onto $\chi_{1,2}(\xi)$:

$$V^{\mu\nu}(\mathbf{r} - \mathbf{r'}) = \frac{e^2}{\kappa} \tau^{\mu}_{\tau_1 \tau_4} \tau^{\nu}_{\tau_2 \tau_3} \int \int \frac{\chi_{\tau_1}(\xi) \chi_{\tau_2}(\xi') \chi_{\tau_3}(\xi') \chi_{\tau_4}(\xi)}{\sqrt{(\xi - \xi')^2 + (\mathbf{r} - \mathbf{r'})^2}} \ d\xi d\xi'. \tag{2}$$

We use notations: τ^0 for the unit matrix, τ^x , τ^y and τ^z , for the Pauli matrices in the layer space and σ^x , σ^y and σ^z , for the Pauli matrices in the spin space. The Coulomb energy (2) is invariant under transformations: $\tau_1 \leftrightarrow \tau_4$, $\tau_2 \leftrightarrow \tau_3$ as well as $(\tau_1\tau_4) \leftrightarrow (\tau_2\tau_3)$. Hence, $V^{\mu\nu}$ is a 3×3 symmetric matrix with indices μ , ν running over a set (0,z,x). If there is a symmetry of the Coulomb interaction under an exchange of layers: $(\xi,\xi') \leftrightarrow (-\xi,-\xi')$ and $1\leftrightarrow 2$ then it restricts further values of the interaction matrix: $V^{0z}=0$ and $V^{zx}=0$. We note also, that $V^{0x}\sim t$, $V^{xx}\sim t^2$ and we neglect it thereafter, whereas $V^{zz}\sim d^2/|z|^3$ as $|z|\to\infty$.

We split the total Hamiltonian (1) into two parts. The first one is invariant under uniform rotations from the SU(4) Lee group in the combined spin and layer space:

$$H^{sym} = \frac{1}{2m} c^{+}_{\alpha\tau p} c_{\alpha\tau p} + \frac{1}{2} \int \frac{d^2q}{(2\pi)^2} V^{00}(q) \exp\left(\frac{-q^2}{4}\right) T^0(q) T^0(-q),$$
 (3)

where (see e.g. [9])

$$T^{\mu}(q) = \sum_{p} c^{+}_{\alpha\tau_{1}p} \tau^{\mu}_{\tau_{1}\tau_{2}} c_{\alpha\tau_{2}p-q_{y}} \exp\{-iq_{x}(p-\frac{q_{y}}{2})\}. \tag{4}$$

Its eigen levels are hugely degenerate. Given any eigen state $|\Psi\rangle_0$ a set of related eigen states can be generated by applying rotations: $|\Psi\rangle = U|\Psi\rangle_0$, where $U \in SU(4)$. For $\nu = 1, 2, 3$ we assume that the ground state is uniform over *p*-orbitals:

$$\Psi = \prod_{i=1}^{\nu} \prod_{p} c_{\alpha_{i}\tau_{i}p}^{+} |empty\rangle.$$
 (5)

Wave-function (5) is an eigen function of the H^{sym} (3). The second anisotropy part of the Hamiltonian (1) is treated like a perturbation:

$$H^{anis} = -c_{\alpha\tau_{1}p}^{+} \left(t \tau_{\tau_{1}\tau_{2}}^{x} + \mu^{z} \tau_{\tau_{1}\tau_{2}}^{z} \right) c_{\alpha\tau_{2}p} - |g| \mu_{B} H c_{\alpha\tau_{p}}^{+} \sigma_{\alpha\beta}^{z} c_{\beta\tau_{p}} + \frac{1}{2} \int \frac{d^{2}\mathbf{q}}{(2\pi)^{2}} V^{\mu\nu}(\mathbf{q}) \exp\left(\frac{-\mathbf{q}^{2}}{4}\right) T^{\mu}(\mathbf{q}) T^{\nu}(-\mathbf{q}).$$
(6)

Here t is the hopping constant. The electrostatic potential μ^z , which is the difference between chemical potentials in the two layers, breaks down the symmetry between the two wells of $V(\xi)$ potential. We assume that the energy of a capacitor formed by the two layers is much lower than the characteristic Coulomb energy: $e^2/\kappa l_H$. The Coulomb energy constants are:

$$E^{\mu\nu} = \int \frac{dz d\bar{z}}{2\pi l_H^2} V^{\mu\nu}(|z|) \exp \frac{-|z|^2}{2} \approx \int \frac{dz d\bar{z}}{2\pi} V^{\mu\nu}(|z|), \tag{7}$$

where the last approximation holds for $(\mu\nu) \neq (00)$ in the limit $d \ll l_H$.

First, we specialize to the SU(4)-symmetric part of the bilayer 2DEG Hamiltonian (3). Weakly non-homogeneous state is generated by a rotation matrix: $c_{\alpha\tau} = U^{\alpha\beta}_{\tau\tau'}(t, \boldsymbol{r})c_{\beta\tau'}$, which adds a gauge matrix field: $\Omega_{\mu} = -i U^{+}\partial_{\mu}U$, in the kinetic energy. An effective low-energy Goldstone Action has an expansion in powers of Ω . We calculated this action following step in step the Ref.[12] for $\nu = 1, 2, 3$ at once:

$$H_G = \frac{E_1}{2} \int \frac{d^2 \mathbf{r}}{2\pi} \left[\operatorname{tr} \left((1 - N)\Omega_{\mu} N \Omega_{\mu} \right) + i \operatorname{sgn}(B^z) \epsilon_{\mu\nu} \operatorname{tr} \left(\Omega_{\mu} \Omega_{\nu} N \right) \right], \tag{8}$$

where $E_1 = E^{00}/2$. The insertion matrices in (8) are non-negative diagonal ones and they represent the occupation number for the electron states:

$$N = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & 0 \end{array}\right),\tag{9}$$

where diagonal blocks are 1×1 and 3×3 in the case $\nu = 1, 3$ and 2×2 in the case $\nu = 2$. It can be proven that $H_G \ge 0$.

The matrices N and 1-N are projector operators that allow only physical rotations into the Hamiltonian (8) which do change the ground state. The vector field Ω_{μ} can be expanded in the basis of fifteen generators of SU(4) Lee group. We subdivide them into two complementary sets: the first one includes generators that do commute with N, constitute an algebra itself and we called it a stabilizer sub-group S; whereas the remaining physical rotations constitute a coset: $U(4)/U(\nu) \otimes U(4-\nu)$, with dimension eight in the case $\nu = 2$ and six in the case $\nu = 1, 3$.

The Hamiltonian (8) is invariant under the time reversal symmetry, which can be chosen as a complex conjugate operator: $U \to U^*$. It follows that $\Omega_{\mu} \to -\Omega_{\mu}^T$. Thus, the time reversal changes the sign of the trace and the sign of the magnetic field B^z in the second term of (8).

The first term in H_G (8) is the gradient energy whereas the second term is proportional to the topological index of a non-homogeneous state:

$$Q = \operatorname{sgn}(B^z) \int \operatorname{curl} \Omega^z \, \frac{d^2 \mathbf{r}}{2\pi} = Z, \tag{10}$$

where Z is the set of integer numbers. The case $Q = \pm 1$ corresponds to the simplest spin skyrmion in the first layer being rotated by a SU(4) matrix to become a general bilayer skyrmion. The energy constant in H_G (8) coincide identically with that of the one-layer case [12], which means that the bilayer skyrmion energy is the same as found for one layer.

We introduce a local bilayer order parameter: $Q(\mathbf{r}) = U(\mathbf{r})NU^+(\mathbf{r})$, very much like magnetization in the theory of magnetism. Rotations from the denominator sub-group S leave Q intact. The total bilayer Hamiltonian in terms of this order parameter reads:

$$H_G = \frac{E_1}{4} \int \operatorname{tr} \left(\nabla Q \nabla Q \right) \frac{d^2 \mathbf{r}}{2\pi} + \operatorname{sgn}(B^z) \frac{E_1}{2} \int \epsilon_{\mu\nu} \operatorname{tr} \left(Q \partial_{\mu} Q \partial_{\nu} Q \right) \frac{d^2 \mathbf{r}}{2\pi}. \tag{11}$$

In this representation the index selection rule (10) is a consequence of the homotopy group identity. Finally, we include the direct Coulomb energy of charge inside a skyrmion core:

$$H_{ee} = \frac{1}{2} \int \int d^2 \mathbf{r} d^2 \mathbf{r'} \frac{\operatorname{curl} \Omega^z(\mathbf{r})}{2\pi} \frac{e^2}{|\mathbf{r} - \mathbf{r'}|} \frac{\operatorname{curl} \Omega^z(\mathbf{r'})}{2\pi}.$$
 (12)

We can cast the anisotropic part of the bilayer Hamiltonian (6) in terms of the order parameter matrix Q as well:

$$H^{anis}/\mathcal{N} = -\left(t + (\nu - 1)E^{0x}\right) \operatorname{tr}(Q\tau^{x}) - \left(\mu^{z} + (\nu - 1)E^{0z}\right) \operatorname{tr}(Q\tau^{z}) - -|g|\mu_{B}H\operatorname{tr}(Q\sigma^{z}) + \frac{1}{2}E^{zz}\left[\operatorname{tr}(Q\tau^{z})\operatorname{tr}(Q\tau^{z}) - \operatorname{tr}(Q\tau^{z}Q\tau^{z})\right],$$
(13)

where \mathcal{N} is the number of degeneracy of the LL, τ^{μ} acts on four-spinor as $\tau^{\mu} \otimes \sigma^{0}$. The Eqs.(11)–(13) defines the effective long-range Hamiltonian of a bilayer at integer ν .

The order parameter can be parameterized by six or eight angles in the case $\nu=1,3$ or $\nu=2$. Actually, not every of those rotations corresponds to a physically distinct eigen state. The total bilayer energy is given by real diagonal matrix elements. One generates all real eigen states from a reference state by rotations from the SO(4) sub-group of the SU(4) group. This group has 6 parameters with two of them being from the stabilizer. Thus, only four global rotations do change the total bilayer energy. We start with the case $\nu=2$ and we use a set of trial many electron wave functions parameterized by the three angles of relevant in our case rotations: θ_{\pm} and ϑ :

$$\prod_{p} U(\vartheta, -\vartheta) R(\theta_{+}, \theta_{-}) c_{+1p}^{+} c_{-2p}^{+} |empty\rangle, \tag{14}$$

where \pm -spin components of electron are first rotated by angles θ_{\pm} , in the layer space and, then, spins in the layer 1,2 are rotated by angles $\pm \vartheta$. Plugging $Q = URNR^+U^+$ into (13) we find:

$$E^{anis}/\mathcal{N} = -E^{zz}\cos\theta_{+}\cos\theta_{-} - (t + E^{0z})\cos\vartheta(\sin\theta_{+} + \sin\theta_{-}) - (\mu^{z} + E^{0z})(\cos\theta_{+} - \cos\theta_{-}) - |g|\mu_{B}H\sin\vartheta(\cos\theta_{+} + \cos\theta_{-}).$$
(15)

The minimum of this energy corresponds to three phases: a) ferromagnetic at $\vartheta = \pi/2$, $\theta_+ = \theta_- = 0$; b) spin singlet at $\vartheta = 0$, $\theta_+ = \pi - \theta_- = \theta$; and c) CAP otherwise, as it is shown on Fig.1. A line of continuous phase transitions between the ferromagnetic phase and CAP is given by:

$$\left[\left(E^{zz} + |g|\mu_B H \right)^2 - \left(\mu^z + E^{0z} \right)^2 \right] |g|\mu_B H = \left(t + E^{0x} \right)^2 \left(E^{zz} + |g|\mu_B H \right). \tag{16}$$

In the spin singlet phase the mixing phase θ , is determined by the equation:

$$(E^{zz}\sin\theta + t + E^{0x})\cos\theta = (\mu^z + E^{0z})\sin\theta. \tag{17}$$

A line of continuous phase transition between the spin singlet phase and CAP is given parametrically by the equation:

$$((t + E^{0x})\sin\theta - E^{zz} + (\mu^z + E^{0z})\cos\theta)(t + E^{0x}) = (|g|\mu_B H)^2\sin\theta,$$
 (18)

whith θ being determined from (17). In the case $\nu = 1, 3$ there is only one phase which is ferromagnetic in both the spin and the layer spaces.

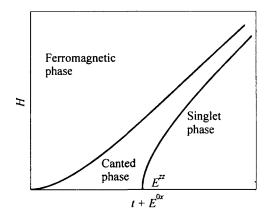


Fig.1. Phase Diagram in the $\nu=2$ gate-symmetric case

Next, we find a skyrmion energy. Skyrmion's order parameter is given by the Belavin – Polyakov (BP) solution for |Q| = 1 [4]:

$$Q_{\rm BP}(z\bar{z}) = \frac{R^2}{R^2 + |z|^2} \left(\frac{|z|^2 |zR|}{\bar{z}R |R^2|} \right), \tag{19}$$

with only one free parameter: the radius of a skyrmion core R. We omit inessential rotation angle between spin and orbital frames arbitrary in the absence of spin-orbit interaction. This Q has to be rotated by a homogeneous matrix RU (see above) in order to minimize the anisotropy energy away from the core. In addition, we allow all homogeneous rotations W from the stabilizer S that transform the BP skyrmion solution (19): $Q(\mathbf{r}) = RUWQ_{\mathrm{BP}}(z\bar{z})W^+U^+R^+$.

We retain only logarithmically divergent spatial integrals and we calculate the minimum of the skyrmion anisotropy energy over the seven free parameters of matrix W: \mathcal{E}_{min}^{skyr} , numerically. Then, we add the direct Coulomb energy (12) and minimize the total skyrmion energy with respect to R:

$$\Delta = \frac{\mathcal{Q} + |\mathcal{Q}|}{2} E_1 + 3 \left(\mathcal{E}_{min}^{skyr} \left(\frac{3\pi^2 e^2}{128\kappa l_H} \right)^2 \log \frac{e^2}{\kappa l_H \mathcal{E}_{min}^{skyr}} \right)^{1/3}. \tag{20}$$

In the case of antiskyrmion Q = -|Q|, the gap consists only from a relatively small anisotropic energy. The total anisotropic skyrmion gap is shown on Fig.2 for the gate symmetric case $\mu^z + E^{0z} = 0$. Note, that the two cusp-like lines coincide with the two

phase transition lines on the Fig.1. A skyrmion in the ferromagnetic phase is a spin-skyrmion with spin rotations being localized in one layer, whereas a skyrmion in the spin-singlet phase is a layer-skyrmion with the electron density being rotated into the other layer.

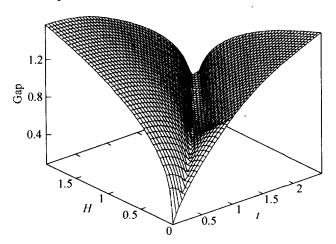


Fig.2. Total anisotropic antiskyrmion gap energy in the $\nu=2$ gate symmetric case

In the case $\nu = 1,3$ we find the minimum of skyrmion's energy to be:

$$\Delta = \frac{Q + |Q|}{2} E_1 + \min\left(2\sqrt{t^2 + \mu_z^2}, \ 2|g|\mu_B H\right). \tag{21}$$

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