CORRELATED WAVEFUNCTION MONTE CARLO STUDIES OF EXCITATIONS IN THE QUANTUM HALL LIQUIDS

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Abstract

Various excitations in the quantum Hall liquid at different Landau level filling factors are studied using a variational quantum Monte Carlo approach. Quantities calculated include spin-flip energies and dispersion relations for the collective modes (the magnetorotons and magnetoplasmons). The present approach goes beyond the lowest-Landau-level and single-mode approximations commonly used in previous studies. The inclusion of Landau-level mixing along with finite-thickness and donor effects satisfactorily explains values for the $\nu = 1$ spin-flip energy that are found in recent photoluminescence experiments on δ-doped samples. In the case of the magnetorotons at $\nu = 1/3$, we show that multiple-mode effects can change the excitation energies significantly, especially for high r_s samples (by nearly 50% at $r_s = 20$).

1. Introduction

Study of quantum Hall liquids provides important insight into the cooperative behavior of electrons, because the ground and excited state properties of these systems are strongly influenced by electron correlations[1]. Previous theoretical investigations[2, 3, 4] of excitations in quantum Hall states at filling factor $\nu = nhc/eB = 1/m$, with $m = 1, 3, \ldots$, have been primarily confined to lowest Landau level analyses. However, in general, the ratio of the Coulomb energy scale to the kinetic energy scale is $(e^2/\epsilon d)/\hbar\omega_c = \nu r_s/2$, which is of order 1 in experimental examples of GaAs quantum wells. Here $\pi d^2 = 1/n = 2\pi l_B^2/\nu$, and r_s is the electron gas parameter, i.e. d in effective atomic units. Hence we expect electrons to pay a kinetic energy cost by mixing in higher kinetic energy orbitals in order to gain correlation energy. This Landau level (LL) mixing is naturally implemented in a variational calculation by using a correlating Jastrow factor Ψ_J.[5, 6]

2. Spin-flip energy at $\nu = 1$

The spin-flip energy (Δ_{SG}) is defined as the discontinuity in the chemical potential $\mu(N)$ at $\nu = 1$. This corresponds to the $k \to \infty$ asymptote of the spin waves discussed

by Kallin and Halperin[2]. Physically, Δ_{SG} can be decomposed as

$$\Delta_{SG} = E_Z + |\Sigma_{\uparrow\uparrow}| - |\Sigma_{\uparrow\downarrow}| + \delta_{KE} \tag{1}$$

where the Σ_{ss} are the exchange-correlation self-energies, E_Z is the Zeeman energy, and δ_{KE} is the discontinuity $\delta\,(\partial E_{kin}/\partial N)$ in the first derivative of the kinetic energy. The terms $\Sigma_{\uparrow\downarrow}$ and δ_{KE} would be 0 in a lowest LL (Hartree-Fock) approximation. Comparison with experiment,[7] as in Figure 2, shows the failure of lowest LL theory: $E_Z \ll \Delta_{SG}^{expt} \ll \Delta_{SG}^{HF}$!

To obtain Δ_{SG} , we construct and optimize variational ground states for $\nu = 1$, $\nu = 1 - \epsilon$ ("hole state"), $\nu = 1 + \epsilon$ ("quasielectron state") and take $\Delta_{SG} = E(N + 1) + E(N - 1) - 2E(N)$, where N electrons would fill the lowest Landau level. The wavefunctions are of the form

$$\Psi = \Psi_J(\mathbf{r}_1 \ldots \mathbf{r}_N)\mathcal{F}_\uparrow(z_{1_\uparrow} \ldots z_{N_\uparrow})\mathcal{F}_\downarrow(z_{1_\downarrow} \ldots z_{N_\downarrow})\,, \tag{2}$$

which, apart from the Jastrow factor, are Laughlin's ground, quasielectron and quasihole states in periodic boundary conditions.[8, 9] Figure 1 shows that the effect of LL mixing (*i.e.* the Jastrow factor) is dramatic, especially in high r_s samples.

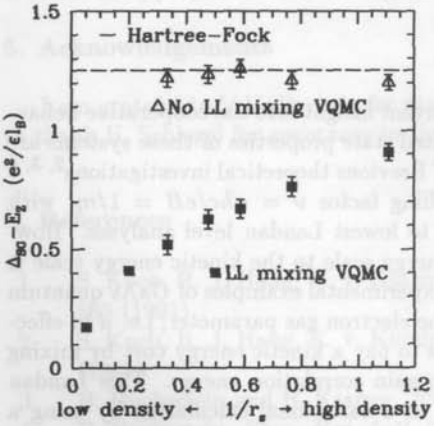

Figure 1. Spin gap in units of the Coulomb energy scale. The dashed line is from Ref. 2

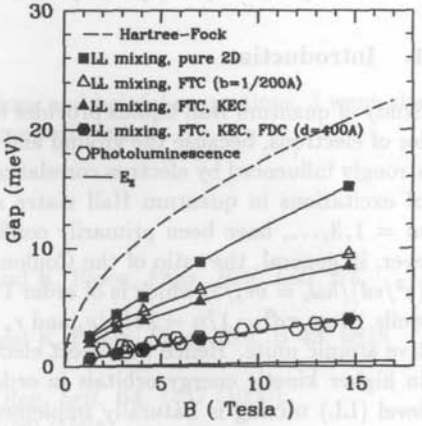

Figure 2. Various corrections to the spin gap: finite thickness (FTC), kinetic energy (KEC), and finite donor distance (FDC) (see text).

A realistic comparison to photoluminescence results[7] requires corrections to the above results. First, the 2D electron liquid has a nonzero thickness, which we have included via a modified Coulomb interaction.[10] This is the finite thickness correction (FTC). Second, the final electron state at the impurity is not infinitely removed from the interface. Hence the "finite distance correction" (FDC). Third, although the first moment of the luminescence line is related to the total energy of the initial state,

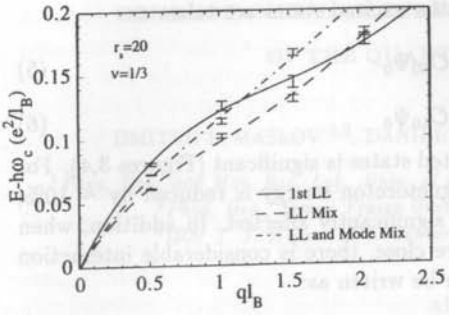

Figure 3. Magnetoplasmon dispersion. The lines are a guide to the eye.

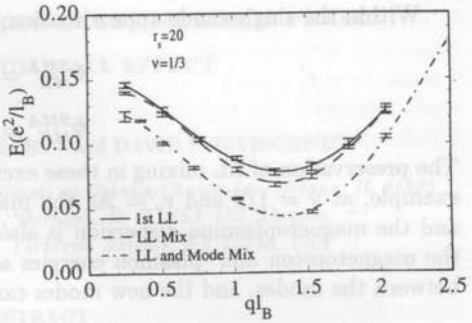

Figure 4. Magnetoroton dispersion.

as described by Apalkov and Rashba[11], their treatment must be modified by an additional term due to the kinetic energy of the electrons[12] if there is Landau level mixing. Hence the "kinetic energy correction" (KEC).

Figure 2 shows the various corrections to the spin-flip energy of a 2D system that are appropriate to interpret Kukushkin and co-workers' experiment.[7] We took the layer thickness to be 100Å, and the impurity distance to be 400Åfrom the interface, both reasonable values. With these parameters, the experimental photoluminescence spectra are well reproduced.

3. Collective Charge Density Excitations

Our treatment of collective charge density excitations, magnetoplasmons and magnetorotons, follows the work of Girvin, MacDonald, Platzman, and Oji[4, 13] which is based on Feynman's theory[14] of excitations in superfluid He^4: the state$\Phi_{\vec{k}} = \rho_{\vec{k}}\Psi_0$ generated by the density operator from the ground state is taken to be an excited state with wavevector $\vec{k}$. Girvin and co-workers decomposed[13, 4] the density operator into a sum of operators projected into Landau levels:

$$\rho_k = \sum_i \sum_{n',n} |n'\rangle_{ii}\langle n|G^{n',n}(k)B_i(k) \,, \tag{3}$$

and then used the (0,0) term to generate magnetorotons and the (0,1) term to generate magnetoplasmons. Since these operators generate excited states that do not contain LL mixing, we use an alternative decomposition[15] in terms of operators

$$\mathcal{O}_{mn}(k) = \sum_j \tau_j(k) \left(a_j^\dagger\right)^m a_j^n \tag{4}$$

that preserve LL mixing. Here $\tau_j(k)$ is the magnetic translation operator acting on the $j-$th particle.

Within the single-mode approximation, the excited states are taken as

$$\Phi_{MR}^{SMA} = \mathcal{O}_{00}\Psi_0 \tag{5}$$

$$\Phi_{MP}^{SMA} = \mathcal{O}_{10}\Psi_0 \tag{6}$$

The preservation of LL mixing in these excited states is significant (Figures 3,4). For example, at $\nu = 1/3$ and $r_s = 20$, the magnetoroton energy is reduced by $\sim 10\%$, and the magnetoplasmon dispersion is also significantly affected. In addition, when the magnetoroton and -plasmon energies are close, there is considerable interaction between the modes, and the new modes can be writen as:

$$\Phi_{MR} = \Phi_{MR}^{SMA} + \alpha\Phi_{MP}^{SMA} \tag{7}$$

$$\Phi_{MP} = \beta\Phi_{MR}^{SMA} + \Phi_{MP}^{SMA} . \tag{8}$$

As seen on Figure 4, mode mixing has a large effect on the lowest excitation energy ($\sim 50\%$ in the roton minimum at $\nu = 1/3$ and $r_s = 20$).

Acknowledgments

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