Interaction of Magnetoexcitons in Two-Dimensional Structures

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The interaction and the formation of bound states of magnetoexcitons in two-dimensional structures with a fully filled Landau level is investigated. A rich spectrum of bound states with a substantial binding energy $e^2/\varepsilon l$ with respect to the cyclotron energy $2\hbar\omega_c$ is found. The dispersion of these states as a function of the total momentum is studied.

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There have recently been several studies of the collective particle-hole excitations in a two-dimensional electron gas in a strong external magnetic field[1] for fully filled Landau levels. These 2D "magnetoexcitons" are very interesting objects in that they exhaust all the spectral weight of the particle-hole excitations; there is no single particle-hole continuum[2] in the excitation spectrum. These excitations also seem to be general in that similar excitations occur for fractionally filled Landau levels[3] and for quasi-2D systems.[2] At any finite temperature, many of these excitations will be thermally excited. It is thus important to understand how the excitations interact with each other.

The magnetoexciton dispersion exhibits a rotonlike minimum at a finite wave vector $q=q_m\cong 2.2l^{-1}$ (l is the cyclotron radius) and hence a local maximum in its density of states at the corresponding energy. A similar local maximum in the density of states is thought to enhance the formation of the two-roton bound state in ^{4}He and the two-phonon bound states in solids[4] even though the question of their existence has not been settled. It is of interest to investigate if a similar bound state exists in the present case.[5] The present problem is much better characterized and simpler numerically; the answer will thus be quite unambiguous. The possible formation of bound states of magnetoexcitons can also be regarded as the formation of a kind of molecule. Molecules formed from excitons that are made from particles in the conduction band and holes in the valence band in strong magnetic fields in 3D systems have been investigated previously[6] in a variational calculation. It is found that exchange is the dominant cause of binding. The present problem is simpler in that the degree of freedom associated with the motion in the z direction is absent. We are thus in a unique position in that we can diagonalize the Hamiltonian directly.

I found a rich excitation spectrum. The lowest excitation occurs with zero momentum, $q=0$, at an energy of $e^2/\varepsilon l$ with respect to the cyclotron energy $2\hbar\omega_c$. For the GaAs heterojunctions, on which the fractional quantized Hall effect has been discovered by Tsui *et al.*, the fully filled condition occurs at a field strength of 50 kG. For this case, $r=(e^2/\varepsilon l)/\hbar\omega_c\cong 0.6$. When r is large, there is strong mixing between Landau levels by the Coulomb energy. The calculation in this paper provides a quantative criterion for when the mixing between the Landau levels will be important.

For $q=0$, the eigenvalues are characterized by the angular momentum n with n even. For $n=0$, two discrete eigenvalues can be discerned. The eigenfunctions for these bound states indicate increased separation of the magnetoexcitons as the binding energy is decreased. On the other hand, there is no particular evidence which indicates an unusually large amplitude with q close to q_m, the rotonlike minimum. This could be due to the large magnitude of the Coulomb interaction at small q, which counterbalances the large density of states at intermediate values of q. An examination of the eigenfunctions for the "unbound" states indicates a large spatial separation of the magnetoexcitons. However, it also exhibits a complicated structure, indicating substantial scattering between them. My result should be measurable experimentally with such techniques as light scattering. Because the energy is quite well separated from integer multiples of the cyclotron energy, there should not be any ambiguity in identifying them. I will now describe the details of the calculation.

The magnetoexciton consists of a particle in the first Landau level separated by a distance q from a hole in the zeroth Landau level, the two moving together with momentum q in a direction perpendicular to their separation. Its wave function in first-quantized form is given by

$$|q\rangle=(1/2N)^{1/2}\sum_j \exp(-\mathbf{q}\cdot\mathbf{C}_j)v_j^\dagger|0\rangle,$$

where one sums over all particles labeled by indices j. Here $|0\rangle$ is the state with lowest Landau level fully filled. C is the center-of-gyration operator.[7] It is like a position operator but does not change the occupation of the Landau levels. $v^\dagger$ is the velocity operator v_x+iv_y. It increases the Landau-level index by 1. From momentum conservation, states with different q are not coupled to

each other. The single-exciton energy is equal to[1]

$$E_{2q}=0.5\left[q\exp\left(\frac{-q^2}{2}\right)+\int_0^\infty dp[1-J_0(pq)](2-p^2)\exp\left(\frac{-p^2}{2}\right)\right]$$
$$=0.5\left(\frac{\pi}{2}\right)^{1/2}\left\{1-e^{-q^2/4}\left[\frac{(1+q^2/2)I_0(q^2/4)-q^2I_1(q^2/4)}{2}\right]+\left(\frac{2}{\pi}\right)^{1/2}qe^{-q^2/2}\right\}.$$

The basis states with two excitons can be formed from a product of these as

$$|q_1,q_2\rangle=(1/2N)\sum_{j\neq l}\exp(-i\mathbf{q}_1\cdot\mathbf{C}_j)\mathbf{v}_j^\dagger\exp(-i\mathbf{q}_2\cdot\mathbf{C}_l)\mathbf{v}_l^\dagger|0\rangle. \quad (1)$$

We have excluded the possibility with $j=1$ where a single electron is excited to the second Landau level. Our basis states are not entirely orthogonal; indeed,

$$\langle q_1,q_2|q_3,q_4\rangle=g=2\pi\delta(q_1-q_3)+2\pi\delta(q_1-q_4)-2\cos[(\mathbf{q}_1\times\mathbf{q}_3+\mathbf{q}_2\times\mathbf{q}_4)/2]/N.$$

Hence it is necessary to solve the generalized eigenvalue problem

$$\sum'_{q_1'}H(q_1,q-q_1;q_1',q-q_1')a(q_1')=E\sum'_{q_1'}\langle q_1,q-q_1|q_1',q-q_1'\rangle a(q_1').$$

I have included only the basis state $|q_1,q_2\rangle$ and not $|q_2,q_1\rangle$ since they are proportional to each other. In my numerical calculation, this is achieved by taking the x axis to lie along the total momentum $\mathbf{q}$ and demanding that $L/2+|q|/2>q_{1x}>|q|/2$ (periodic boundary condition assumed). This restriction is indicated by the prime over the sum in the above equation. The single-particle part of the Hamiltonian, $\sum_j v_j^2/2m$, provides for a constant term $2\hbar\omega_c$. I shall measure the energy with respect to this from now on. The Hamiltonian is then just the Coulomb potential $H=\sum_{i>j}r_{ij}^{-1}$, where $r^{-1}=\int d^2p\,v(p)\exp(i\mathbf{p}\cdot\mathbf{r})$; $v(p)=(2\pi p)^{-1}$. The Hamiltonian matrix coupling two magnetoexcitons with each other is a sum of the pairwise interaction between the individual constituents that make up the excitation, viz.

$$\langle q_1,q_2|H|q_3,q_4\rangle=V(12,34)+V(21,34)+V(12,43)+V(21,43),$$

where

$$V(12,34)=\int d^3p\exp(-p^2/2)v(p)\{S'(p,-p+q_2-q_3,q_1-q_4)$$
$$\times\exp[i\mathbf{p}\times(\mathbf{q}_2+\mathbf{q}_3)/2-i\mathbf{q}_1\times\mathbf{q}_4/2-i\mathbf{q}_2\times\mathbf{q}_3/2](1-|p|^2/2)$$
$$+S'(q_1-q_4,q_2-p,p-q_3)|p|^2\exp[i\mathbf{p}\times(\mathbf{q}_2-\mathbf{q}_3)/2-i\mathbf{q}_1\times\mathbf{q}_4/2]/2\}. \quad (2)$$

Here S' is a three-particle correlation function defined by

$$S'(a,b,c)=(1/N)^2\sum_{l\neq i\neq j}\langle 0|\exp(i\mathbf{a}\cdot\mathbf{C}_i)\exp(i\mathbf{b}\cdot\mathbf{C}_j)\exp(i\mathbf{c}\cdot\mathbf{C}_l)|0\rangle.$$

When the Landau level is fully filled, the excitations in Eq. (1) involve the velocity operators $v^\dagger$. In the calculation of the Hamiltonian matrix elements, they need to be paired up with their Hermitian conjugates. Thus the six different electron labels in the matrix element get paired up and only three-point functions are necessary. For a partially filled Landau level, no velocity operators are present and a six-point function may be necessary. The three-point function is quite difficult to calculate for a partially filled band. For a filled band, they can be computed exactly as

$$S'(a,b,c)=[(2\pi)^2\delta(\mathbf{b})\delta(\mathbf{c})-2\pi\delta(\mathbf{a})-2\pi\delta(\mathbf{b})-2\pi\delta(\mathbf{c})+\exp(i\mathbf{a}\times\mathbf{b}/2)+\exp(-i\mathbf{a}\times\mathbf{b}/2)]/N.$$

Substituting this expression for S' back into Eq. (2) I obtain

$$V=\exp[-i\mathbf{q}_2\times\mathbf{q}_3+\mathbf{i}q\times(\mathbf{q}_3-\mathbf{q}_2)/2]$$
$$\times[E(q_2)2\pi\delta(q_2-q_3)+f_3(q_2,\tfrac{1}{2})+f_3(q_3,\tfrac{1}{2})-\exp(-q_2^2/2)|q_2|/2-\exp(-q_3^2/2)|q_3|/2+(\pi/2)^{1/2}/2]/N$$
$$-\exp[i\mathbf{q}\times(\mathbf{q}_3-\mathbf{q}_2)/2-(q_3-q_2)^2/2](1-|(q_3-q_2)|^2/2)/|\mathbf{q}_3-\mathbf{q}_2|N$$
$$+\exp[i\mathbf{q}\times(\mathbf{q}_3-\mathbf{q}_2)/2]f_2(q_3-q_2,\tfrac{1}{2}) \quad (3)$$

where

$$f_3 = f_1 - f_2/2,\quad f_1(q,a) = 0.5(\pi/a)^{1/2} I_0(q^2/8a)\exp(-q^2/8a),$$

$$f_2(q,a) = 0.5(\pi/a)^{1/2}\exp(-q^2/8a)[I_0(q^2/8a)(0.5/a - q^2/8a^2) + I_1(q^2/8a)q^2/8a^2].$$

The special case $q=0$ is particularly instructive. One can exploit the rotational symmetry to simplify the problem and reduce the number of degrees of freedom to one. This will serve as a standard by which we can gauge the convergence of the calculation for finite q, which is much more difficult numerically. The Hamiltonian in the subspace of angular momentum n is thus given by

$$H' = \pi\{E(q_2)\delta(|q_2| - |q_3|)/q_2 - f_5(q_2,q_3,n) + f_4(q_2,q_3,n) + J_n(q_2q_3)[f_3(q_2,\tfrac{1}{2}) + f_3(q_3,\tfrac{1}{2}) - \exp(-q_2^2/2)|q_2|/2 - \exp(-q_3^2/2)|q_3|/2 + (\pi/2)^{1/2}/2]\}/N + (\mathbf{q}_2 \to -\mathbf{q}_2),$$

where

$$f_4(q_2,q_3,n) = \int_0^\infty J_n(pq_3)J_n(qp_2)\exp(-p^2/2)p^2\,dp,$$

$$f_5(q_2,q_3,n) = 2\int_0^\pi d\theta(|\mathbf{q}_2 - \mathbf{q}_3|^{-1} - |\mathbf{q}_2 - \mathbf{q}_3|/2)\exp(-|\mathbf{q}_2 - \mathbf{q}_3|^2/2)\cos(n\theta).$$

There cannot be any state for odd n because $\mathbf{q}_3 \to -\mathbf{q}_3$ should produce the same state! In general f_4 can be written down in terms of special functions.[8] The resulting expression is not very convenient computationally. I have thus evaluated the integral numerically. A mesh size of $\delta p = 0.4$ and an upper limit $p=5$ is found to be adequate. For $q_2 = q_3 = 0$, $f_4 = (\pi/2)^{1/2} = 1.2533$. Our numerical results agrees with this value to within 1%.

In the same spirit, the overlap matrix element can also be expressed for circularly symmetric states.

I have diagonalized the matrix with the overlap in two ways. First, I diagonalize the equation with the EISPACK subroutines. The basis set is overcomplete. This overcompleteness could cause a numerical problem in that the subroutine may become unstable. This instability does not arise provided the mesh is small enough (0.05) and the range of q_1 is not too big (<4). Second, I have diagonalized the overlap matrix, discarded those basis states with zero eigenvalues since they correspond to the overcomplete set, and reexpressed the Hamiltonian in terms of the eigenfunctions corresponding to the nonzero eigenvalues of the overlap operator. The "renormalized" Hamiltonian is then diagonalized. The lowest seven eigenvalues for the zero-angular-momentum manifold for $\delta q = 0.1$ and $q_{\max} = 16$ are -0.97, -0.63, -0.39, -0.26, -0.18, -0.12, -0.075. Note that the two-particle density of states at $q=0$ is essentially the Raman spectrum.[4] I have examined the density of states of my calculation. In addition to the bound states, I found that the "continuum" is quite spread out up to 3.7 with a peak at an energy of 3.

The renormalized wave function $g(q)$ for the lowest two eigenstates is shown in Fig. 1. These wave functions exhibit oscillations with a period that is the inverse of the average separation between the magnetoexcitons. As the state becomes less bound, the period shortens, indicating that the magnetoexcitons are further apart. The damping of the wave functions in q space becomes less as the state becomes less bound. The wave function for a state with an energy in the "continuum" region exhibits rapid oscillation close to the origin. The damping, if any, is very slow in q space.

At $q=0$, my basis states in Eq. (1) are also coupled to the ground state. I found that the change in energy of the state $|q_1, -q_1\rangle$ due to the coupling to the ground state is at most $(r/22)(e^2/\varepsilon l)$. The second-order correction to the ground-state energy is equal to $(r/16)e^2/\varepsilon l$. These are small numbers in the weak coupling limit of small r.

For a finite q, the angular momentum is no longer a good quantum number; I have to diagonalize the full 2D Hamiltonian instead. Because of the increase in dimension, it is not possible to perform a calculation numeri-

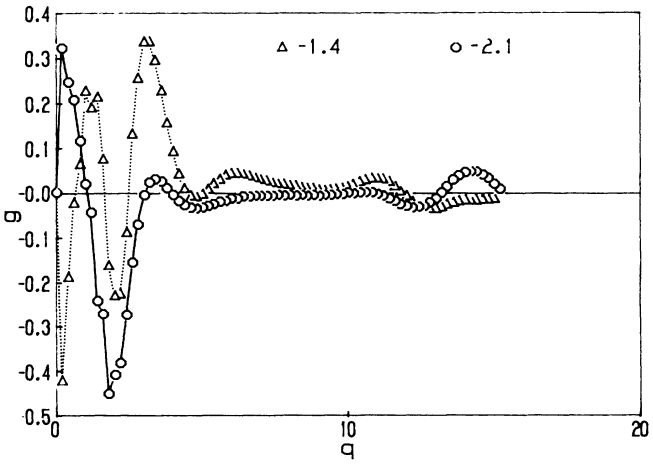

FIG. 1. The wave function $g(q)$ as a function of q for the lowest two eigenvalues for $q=0$ and $l=0$.

cally as accurate as for the case with $q=0$. The Hamiltonian is still symmetric with respect to a reflection with q as the mirror line. Once this symmetry is incorporated, the Hamiltonian turns from a complex Hermitian operator to a real symmetric operator. This saves the required computer memory by a factor of 4. With a mesh size $\delta q_{x(y)}=0.25$ and a maximum deviation from q, $\Delta q_{x(y)}=5$, I have diagonalized the 2D Hamiltonian. For $q=0$ the lowest eigenvalue is -1. This is within 2% of the lowest eigenvalue that I have obtained for the $l=0$ solution and I consider this a reasonable compromise between numerical accuracy and efficiency. The eigenfunctions agree qualitatively with that from the $l=0$ solution. However, because of the square-boundary condition that I have imposed the eigenfunctions are no longer circularly symmetric. It is also much more difficult to separate the discrete from the continuous spectrum for two reasons. First, all the eigenvalues of the different angular momentum components now have entered into the picture and this creates an impression of a dense set in those regions where the eigenvalues are discrete. Second, limited by the size of the computation I am unable to investigate as wide a range of q as for the $l=0$ calculation. The continuum states are usually quite spread out in q space. Their eigenvalues are changed by the boundary effects. The lowest eigenvalue is still easily identifiable, however. I found the lowest eigenvalues to be equal to -1, -0.72, -0.665, -0.643 for $q=0$, 0.5, 1, 1.5, respectively. There is thus a dispersion at small q which then flattens out.

To summarize, I have studied the interaction between magnetoexcitons and found a rich spectrum of bound states. These states should be measurable experimentally. Corresponding bound states may also exist in quasi 2D structures and remain to be investigated. In this paper, I have assumed that the external magnetic field is so strong that all spins are lined up. The above calculations can be extended to include the effect of spins similar to the calculations of Kallin and Halperin.[1]

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[2]S. T. Chui, unpublished.

[3]S. M. Girvin, A. H. MacDonald, and P. M. Platzman, Phys. Rev. Lett. **54**, 581 (1985).

[4]See, for example, P. A. Fleury, in *Dynamical Properties of Solids,* edited by G. K. Horton and A. A. Maradudin (North-Holland, Amsterdam, 1980), Vol. 3, and references therein.

[5]J. Quinn and co-workers have also performed an independent study of the possibility of bound states of magnetoexcitons (unpublished).

[6]S. T. Chui, Phys. Rev. B **9**, 3438 (1974).

[7]See, for example, R. Kubo, S. J. Miyake, and N. Hashitsume, in *Solid State Physics Vol. 17,* edited by F. Seitz and D. Turnbull (Academic, New York, 1965); see also S. M. Girvin and T. Jach, Phys. Rev. B **29**, 5617 (1984).

[8]From formula 6.633 of I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965). We get, for example, for $n=0$,

$$f_4=0.7071\sum_{m=0}^{\infty}\Gamma(m+\tfrac{3}{2})(-q_3^2/2)^m \times F(-m,-m,1,q_2^2/q_3^2)/m!^2.$$