Variational Monte Carlo calculation of the spin gap in the \( \nu = 1 \) quantum Hall liquid

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A variational method of calculating the spin 1 excitation energies of the \( \nu = 1 \) quantum Hall liquid is presented in detail. We are able to include Landau-level mixing and finite-thickness effects. The many-body wave functions of the states near \( \nu = 1 \) filling are taken to be a product of a lowest-Landau-level Laughlin-type wave function and a Jastrow factor. A significant reduction in the calculated spin gap is found due both to Landau-level mixing (\( \sim 40\% \)) at \( r_s = 1 \) and to the effect of the finite thickness of the liquid (a further \( \sim 30\% \)) at \( r_s = 1 \). We find our calculations to be consistent with recent photoluminescence experiments in \( \delta \)-doped samples. [S0163-1829(97)06331-5]

The excitation spectrum of quantum Hall systems\(^1\) has been an active area of both theoretical and experimental research ever since their discovery. The study of these systems is difficult both because the experiments are difficult to perform and to interpret, and because of the mathematical difficulties that arise in the existing theories. Even in the presently studied case of the lowest-energy (spin) excitations in the integer quantum Hall systems, which are qualitatively understandable semiclassically, quantum corrections are so important that experimental\(^2\)–\(^4\),\(^6\) and theoretical\(^5\)–\(^9\),\(^11\) determinations of the fundamental spin gap are as much as a factor of 2 off from each other.

Within the framework of Hamiltonian quantum mechanics, single-spin excitations (\( S = 1 \)) have been studied using perturbation theory,\(^10\) the Hartree-Fock formalism,\(^7\)\(^9\) and the random phase approximation.\(^11\) Using Chern-Simons Landau-Ginzburg theory, it is possible to study spin-texture excitations, i.e., Skyrmions.\(^8\) In addition, numerical diagonalizations of small systems have also been carried out.\(^12\) Recently, we briefly presented variational results on the \( S = 1 \) excitation energies.\(^13\)

In this paper we develop in detail a variational method to obtain \( S = 1 \) excitation energies of the \( \nu = 1 \) quantum Hall liquid. The approach is based on the observation that following Laughlin’s work\(^14\) and working within the framework of a single-spin flip, we are able to write down nearly exact wave functions for both the ground and excited states of the system in question. Techniques used to study correlations in the homogeneous electron gas\(^15\) can be extended to the quantum Hall liquid to improve on Laughlin’s wave functions. Monte Carlo integration techniques make the evaluation of the required variational integrals feasible for large enough systems (up to 100 electrons per unit cell under periodic boundary conditions) for the properties of infinite systems to emerge.

The organization of this paper is as follows: In Sec. I, we describe the formalism and the variational wave functions used. In Sec. II, we present the details of the Monte Carlo method used to evaluate the variational integrals. In Sec. III, the results for the \( \nu = 1 \) quantum Hall system are given. Section IV addresses the issue of the finite thickness of the experimentally realizable two-dimensional (2D) electron systems. In Sec. V, we compare our predictions for the spin gap at various carrier densities to photoluminescence experiments. We conclude in Sec. VI.

I. FORMALISM

The full many-body Hamiltonian for charged particles in two dimensions in a constant perpendicular magnetic field \( B \) is

\[
H = \sum_i \frac{\hbar^2}{2m^*} \left( \mathbf{p}_i - \frac{q}{c} \mathbf{A}(\mathbf{x}_i) \right)^2 + \sum_{i<j} V(|\mathbf{x}_i - \mathbf{x}_j|),
\]

where \( m^* \) is the effective mass of the particles (in our case the effective mass of electrons in the GaAs conduction band), \( q \) is their charge, and \( V(r) \) is the interparticle potential. Both the pure Coulomb and the finite-thickness-modified potentials are studied. \( \mathbf{A} \) is the vector potential corresponding to the perpendicular \( \mathbf{B} \)-field \( B_z \) with \( \mathbf{A} = (-yB,0) \) in the Landau gauge.

For a 2D plane with a perpendicular magnetic field \( B \), in the absence of interparticle interactions the single-particle states form highly degenerate Landau levels (LL’s). The energies of the Landau levels are \( E_1 = 1/2h\omega_c - 1/2E_Z \), \( E_2 = 1/2h\omega_c + 1/2E_Z \), \( E_3 = 3/2h\omega_c - 1/2E_Z \), etc., where \( \omega_c = eB/m^*c \) is the cyclotron frequency, \( E_Z = g_L\mu_B B \) is the Zeeman energy, \( g_L \) is the Landé Landé factor, and \( \mu_B \) is the Bohr magneton. The characteristic length of the single-particle states is the magnetic length, \( l_B = \sqrt{\hbar c/eB} \). The degeneracy of the Landau levels can be expressed as \( (2\pi l_B^2)^{-1} \) per unit area. We introduce the usual 2D dimensionless density parameter \( r_s \), given by \( n = (\pi r_s^2 a_0^2)^{-1} \), where \( n \) is the particle density, \( a_0 \) is the effective Bohr radius, \( a_0 = \hbar^2/\epsilon m^* \), and \( \epsilon \) is the macroscopic dielectric constant. In terms of \( r_s \), the filling factor \( \nu \) is given as \( \nu = 2(1/l_B/a_0)^2 \). The spin gap is defined as the discontinuity in the chemical potential \( \mu \) across the \( \nu = 1 \) state. In the noninteracting picture, this gap \( \Delta_{SG} \) is simply given by the Zeeman energy \( E_Z \) computed at the magnetic field required for the Landau-level degeneracy to equal the number of carriers in the sample. However, the experimental value is much larger.
The Hartree-Fock approximation, discussed below, includes exchange effects, which open up the gap to a value significantly larger than experiment. The corrections discussed in this paper reduce the Hartree-Fock gap and give good agreement with experiment.

For a finite particle number simulation, such as ours, we can write the above as

$$\Delta_{\text{SF}} = \partial E(N,B)/\partial N |_{\nu = 1 + \epsilon} - \partial E(N,B)/\partial N |_{\nu = 1 - \epsilon}.$$

(2)

For completeness, we give the details of the form of the many-body wave function.

A. The $\nu=1$ ground state in the lowest Landau level

We start our discussion with the $\nu=1$ ground state. Neglecting LL mixing, the correct wave function to use is completely determined by the Pauli exclusion principle to be a Slater determinant of all of the available single-particle states within the first Landau level. This state is nondegenerate. The functional form of the Slater determinant is in turn completely determined by the Pauli exclusion principle to be a complex parameter that describes the shape of the simulation cell. For notational convenience we will assume positive particles throughout this paper. The parameters $K_0$ and $Z_0$ can be freely chosen subject to the above constraints, without an effect on the total energy.

The special property of $\Psi_{\text{ground}}/\Pi_{i=1}^{N_s} \exp(-y_i^2/2l_B^2)$ is that it is the only analytic function of the particle coordinates $z_i$ that satisfies periodic boundary conditions appropriate in a magnetic field for $\nu=1$ filling; the analyticity of the function ensures that the wave function is fully contained in the lowest Landau level. $\Psi_{\text{ground}}$ has the property that, for the $N \to \infty$ limit, the charge density is constant. Even for the finite cells studied, the charge inhomogeneity is imperceptible.

B. The quasihole state

To construct the quasihole state, we consider the full Landau level with one particle removed. We keep the parameters $\phi_a$ and the simulation cell the same as in the case of the ground state. This amounts to keeping the magnetic field and therefore the flux through the unit cell fixed at $N_t$. The quasihole (QH) state is in fact the ground state of this $N_t - 1$-particle system. Following Haldane and Rezayi, we take

$$\Psi_{\text{QH}} = F^{\text{cm}} \left( \sum_{i=1}^{N_s-1} z_i \prod_{k=1}^{N_s-1} \exp \left( -\frac{y_k^2}{2l_B^2} \right) \prod_{i<j} \partial_1 \left[ \pi(z_i - z_j)/L_1 \right], \right.$$

$$\left. \times \theta_1 \left[ \pi(z_k - \bar{z})/L_1 \right] \right)$$

(9)

where $F^{\text{cm}}(Z) = \exp(iK_0Z) \theta_1 \left[ \pi(Z - Z_0)/L_1 \right]$, and $Z = \sum z_i$, with $z_i = x_i + y_i$ complex numbers representing the 2D Cartesian coordinates of the particles and $\theta_1$ is the odd elliptic $\theta$ function. The corresponding wave function for (negatively charged) electrons is given by replacing $z$ with $z^*$ throughout. For notational convenience we will assume positive particles throughout this paper. The parameters $K_0$ and $Z_0$ can be freely chosen subject to the above constraints, without an effect on the total energy. The charge density in this state is not uniform, because there is a unit charge deficiency at the location of the hole. The location of the hole, $\bar{z}$ is not a dynamical variable in the simulation. $\bar{z}$ may be set to an arbitrary location—it does not affect any of the physical quantities calculated. The local filling factor is $1$ except in the direct vicinity of the hole.
C. The quasiparticle state

The quasiparticle (QP) state is constructed in analogy to the quasihole state: We add the extra particle \((z_{N+1})\) in an arbitrary single-particle state, without symmetrizing with the other particles:

\[
\Psi_{\text{QP}} = \Psi_1'(z_{N+1})\Psi_{\text{gnd}}(z_1, \ldots, z_N),
\]

where

\[
\Psi_1'(z) = \exp(i\kappa z)\exp\left(-\frac{y^2}{2l_B^2}\right) \prod_{i=1}^{N} \partial_1[\pi(z - \zeta_i)/L_1|\tau]
\]

and the parameters \(\kappa\) and \(\zeta_i\) are constrained by

\[
\exp(i\kappa L_1) = (-1)^N \exp(i\phi_1),
\]

\[
\exp\left(2\pi i \sum_k \zeta_k/L_1\right) = (-1)^N \exp(i\phi_i - i\kappa L_1\tau).
\]

Symmetrization is not necessary because the \((N+1)\)th particle is in the reversed-spin state. The freedom in the choice of the parameters \(\kappa\) and \(\zeta_i\) is related to the degeneracy of single-particle states in a Landau level: they specify which single-particle state the flipped-spin particle occupies. The energy of the quasiparticle state is independent of these parameters so they are chosen arbitrarily for convenience. Similarly to the quasihole state, the quasiparticle state is also inhomogeneous, having one unit of excess charge in the vicinity of the quasiparticle.

D. Landau-level mixing

Following earlier work on the effect of Landau-level mixing on the ground state energies of quantum Hall liquids and Wigner crystals, we introduce correlations into the system with the use of a Jastrow factor:

\[
\Psi_{\text{correlated}} = \Psi_1'\Psi_{\text{LLL}},
\]

where the \(\Psi_{\text{LLL}}\) are the lowest-Landau-Level wave functions defined above. The form of the Jastrow factor we use is

\[
\Psi_J = \prod_{i<j} e^{-u(|r_i - r_j|)}.
\]

We choose for the pseudopotential \(u\) the variational form

\[
u(r) = -\frac{A}{\sqrt{r}} \left[1 - \exp\left(-F_r r - \frac{F^2}{2} - \frac{F^3}{12}\right)\right].
\]

A and \(F\) are variational parameters constrained by the cusp condition:

\[
AF^3 = \frac{1}{4} \begin{cases} 1 & \text{opposite spin} \\ \frac{1}{3} & \text{same spin}. \end{cases}
\]

This equation shows that we use different forms of the pseudopotential \(u\) to correlate same spins and opposite spins.

The cusp condition is equivalent to imposing that the many-body wave function behave as a true eigenstate of the full Hamiltonian in the limit in which two particles are finitessimally close to each other. For a detailed discussion of the cusp condition and the changes in the form of the pseudopotential for the finite thickness case, see Appendix A.

The inclusion of the Jastrow factor introduces a difference between the per-particle kinetic energy of the three states, and hence makes it necessary to include kinetic energy effects in the calculation of the spin gap. Changing from lowest-Landau-level wave functions to wave functions including Landau-level mixing will affect the interparticle energy contributions to the spin gap as well. Our calculation proceeds in two stages: first we minimize the total energy of the three states under study with respect to the Jastrow parameters \(A\) and \(F\), and then we use these parameters to determine the second difference of the total energies.

II. COMPUTATIONAL METHOD

The variational quantum Monte Carlo (VQMC) method has been shown to be highly accurate in evaluating total energies of semiconductors and of jellium systems. Fixed-phase stochastic calculations have shown that a variational form of the Jastrow factor similar to ours used by Price et al. captures about 75% of the absolute correlation energy due to Landau-level mixing in quantum Hall systems at filling \(\nu = 1/3\). We expect the ratio to be similar at \(\nu = 1\). Since the systems at \(\nu = 1\), \(\nu = 1 + \epsilon\) and \(\nu = 1 - \epsilon\) are very similar, the error we make in evaluating the energies can be assumed to be very similar in the three states studied, and the spin gap, which depends on energy differences between these states, is not expected to be very sensitive to this error. The accuracy of the method and the expected cancellation of the errors make it possible to take second differences of the variational energies and obtain meaningful results. Ultimately, as discussed below, the reliability of our results is demonstrated by matching exact analytical calculations in the appropriate limits. These limits will be discussed in the section on Results.

The VQMC method is based on the stochastic evaluation of the variational integral

\[
E = \frac{1}{\langle \Psi | \Psi \rangle} \int dR \frac{\Psi^*(R) H \Psi(R)}{\Psi(R)},
\]

where \(R\) stands for the \(2N_{el}\)-dimensional variable \((r_1, r_2, \ldots, r_{N_{el}})\) specifying the particle configuration. This equation can be rewritten

\[
E = \int \frac{H\Psi(R)}{\Psi(R)} d\mu(R) = \lim_{n \to \infty} \sum_{k=1}^{n} \frac{H\Psi(R_k)}{\Psi(R_k)},
\]

where

\[
d\mu(R) = |\Psi(R)|^2 dR.
\]
Here $n$ is the number of sample configurations taken. The “local energy” $[H\Psi(R)]/\Psi(R)$ is evaluated at each step of a random walk of the particle configuration $R_i$, and averaged. The walk is guided by the value of $|\Psi|^2$, i.e., the algorithm is designed so that any particle configuration is visited with probability density $|\Psi|^2$. In our study, we consider only one system—in other words, we use the ergodic assumption to equate ensemble averages to time averages. Each run typically consists of ten repetitions, each repetition consisting of 100 warm-up cycles and 1000 averaging cycles. Each cycle involves updating the position of all of the particles in turn.

The guiding of the walk is performed according to the algorithm given by Fahy, Wang, and Louie. In this scheme particles are displaced with probability $P = \min[1, |\Psi(R_{\text{new}})|^2/|\Psi(R_{\text{old}})|^2]$. This probability only depends on the ratio of the new and old wave functions. Since our wave function is a product over particles and particle pairs, the above ratio can be evaluated substantially faster than the ratio of two wave functions of a general form.

### A. Kinetic Energy

The “local energy,” that is the value $H\Psi/\Psi$ sampled at every step of the walk, is a sum of kinetic and potential terms. The kinetic energy per particle is simply given by $\hbar^2(\nabla_i + ie A(r_i) / \hbar c)^2 \Psi / 2m^*$ where

$$K_i = -\frac{\hbar^2}{2m^*} \left[ \frac{(\nabla_i + ie A(r_i) / \hbar c)^2 \Psi}{\Psi} \right] = 2T_i - |F_i|^2,$$

where

$$F_i = \sqrt{\frac{\hbar^2}{2m^*} \left( \nabla_i \ln \Psi + \frac{ie A(r_i)}{\hbar c} \right)}.$$  

and

$$T_i = -\frac{1}{2} \frac{\hbar^2}{2m^*} \nabla_i^2 \ln \Psi - \frac{|F_i|^2}{2}.$$

Here $\nabla_i$ denotes differentiation with respect to $r_i$. Note that $\mathbf{F}$ is a vector quantity and the expression $|F|^2$ denotes the dot product $\mathbf{F}^* \cdot \mathbf{F}$. Green’s theorem shows that

$$\langle K_i \rangle = \langle |F_i|^2 \rangle = \langle F_i \rangle = \langle \text{kinetic energy} \rangle.$$  

Since $K_i \neq T_i \neq |F_i|^2$ at a general point in configuration space, sampling all three of $K_i$, $T_i$, and $|F_i|^2$ provides an independent check for the internal self-consistency of the program. An additional advantage of writing the kinetic energy in terms of $T$ and $F$ is that multiplicative factors (i.e., the Jastrow factor) in the wave function can be treated separately:

$$\nabla_i \ln \Psi = \sum_{j \neq i} -\nabla_i u(r_i - r_j) + \nabla_i \ln \Psi_{\text{LLL}},$$

$$\nabla_i^2 \ln \Psi = \sum_{j \neq i} -\nabla_i^2 u(r_i - r_j) + \frac{1}{l_B^2}.$$  

### B. Potential Energy

The potential energy of the quantum Hall liquid arises from the Coulomb interaction between the electrons. We also include a positive neutralizing background to avoid the infinities associated with the long-ranged potential. In the periodic boundary condition scheme that we adopt, the total potential energy per simulation cell is given by

$$E_{\text{pot}} = E_{e-e} + E_{e-b} + E_{b-b},$$

where

$$E_{e-e} = \frac{e^2}{2} \sum_{j \neq i} \nu(|r_i + R - r_j|)$$

and

$$E_{e-b} + E_{b-b} = -\frac{e^2 N_e^2}{2V} \int d^2 r V(r).$$

Here $V$ stands for the volume of the simulation cell and $\nu(r)$ is the electron-electron potential. $R$ are the lattice vectors defining the simulation cell, and $r_i$ are the two-dimensional coordinates of the particles inside the simulation cell. The prime over the sum means that self-interaction terms (i.e., terms with $i = j$ and $R = 0$) are not included. Interactions of the particles with their own images in other simulation cells are included following Ref. 20. We performed calculations both for Coulombic interactions and for a model interaction that includes finite-thickness effects. The finite thickness case will be discussed in detail below.

In order to compute the potential energy, we use a generalization of the Ewald summation method. This technique allows the efficient evaluation of the potential energy by performing the sums partly in real space and partly in Fourier space. The potential energy is given by

$$E_{\text{pot}} \sum_{G} \rho_G^* h(G) + \frac{e^2 N_e^2}{2V} \sum_{j \neq 0} w(|r_i + R - r_j|),$$

where

$$\rho_G = \frac{(2\pi)^N}{V} \sum_{j=1}^N e^{iG \cdot r_j}$$

and where $H$ is a constant and $w(r)$ and $h(G)$ are short-ranged functions. The $G$ are reciprocal lattice vectors of the simulation cell. The expressions for $w(r)$ and $h(G)$ along with their derivations are given in Appendix B.

### C. Finite-size scaling

We checked the convergence of our results with respect to the size of the simulation cell up to a cell size of 100 electrons. We find a slightly different scaling behavior for the
cases of correlated and lowest-Landau-level wave functions. For the case of no Landau-level mixing, the finite-size effect is dominated by the self-interaction of the quasielectrons and quasiholes with their own images in the other cells. For the uncorrelated system, the quasiparticles and holes can be approximated by well-localized charges entirely contained in one unit cell. The finite-size effect here can therefore be approximated by a Coulombic term that scales as $1/\sqrt{N_{\text{el}}}$. This scaling is given in Fig. 1.

The finite-size scaling for the correlated case (Fig. 1) is dominated by kinetic energy effects. Essentially, the quasiparticles are not fully contained in smaller simulation cells because of the correlations introduced by the Jastrow factor. To account for finite-size effects here, we increased the cell size until the change in our result was within the statistical error of the calculation ($N_{\text{el}}=50\cdots100$), i.e., no extrapolation was used. The spin gap data reported in this paper correspond to a 50-electron simulation.

### III. RESULTS

The effect of Landau-level mixing on the states can be conveniently described in terms of the pair distribution function $h(r)$ (Fig. 2). We define $h$ as

$$h(r) = \frac{(N_{\text{el}}-1)}{N_{\text{el}}} V_{\text{cell}} \int d\mathbf{r}_1 \cdots d\mathbf{r}_{N_{\text{el}}}$$

$$\times \frac{1}{N_{\text{el}}(N_{\text{el}}-1)} \sum_{i < j} \delta(\mathbf{r}_i - \mathbf{r}_j) |\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_{\text{el}}})|^2.$$  

(32)

The normalization factor is chosen to ensure that $h(r)$ integrates to $(N_{\text{el}}-1)V_{\text{cell}}/N_{\text{el}}$ in the simulation cell for the case of $\Psi$ normalized to 1. $h(r)$ describes the probability distribution of particles at a distance $r$ from a test particle. In other words, $h(r)$ describes the shape of the exchange-correlation hole around the test particle. For an infinitely large simulation cell, the normalization condition translates to $h(\mathbf{r} \to \infty) = 1$, since the total volume of the exchange-correlation hole around a particle is exactly 1.

In the dense limit ($r_s \to 0$) kinetic energy effects dominate the electron-electron interactions, and therefore we expect the system to behave as if restricted to the lowest Landau level. In this case, the spin gap is given by the exchange energy of a particle in the system in addition to the Zeeman energy. In the quasiparticle state, the presence of a flipped-spin particle causes the pair distribution function to be finite at zero separation. For a simulation cell with $N$ particles at $\nu = 1$, the quasiparticle state ($N+1$ particles per unit cell) pair distribution function takes the value $1/N$ at $r=0$. The Coulomb energy cost associated with this change in $h(r)$ is the spin gap minus the Zeeman energy.

The introduction of the Jastrow factor describes the dynamical correlation of the electrons because of the Coulomb repulsion between the particles. For all three states the exchange-correlation hole deepens, and the pair distribution function diminishes near $r=0$. The effect is most dramatic for the quasiparticle state. As the pair distribution functions of the states at $\nu = 1 \pm \epsilon$ become more similar, the potential energy difference between them is reduced. The effect of filling factor and correlation on the pair correlation function is shown in Fig. 2.

The neglect of Landau-level mixing in the states near $\nu = 1$ is equivalent to the Hartree-Fock approximation taken by Kallin and Halperin.\textsuperscript{7} They showed analytically that the spin gap is given by $\sqrt{\pi/2}$ in units of $e^2/\epsilon l_B$ in addition to the Zeeman energy. We were able to reproduce this result by simply switching off the Jastrow factor and applying the finite-size scaling scheme described in the previous section (see Fig. 1 in Ref. 13).

The effect of the Jastrow factor is to decrease the gap dramatically. At typical densities ($r_s = 2$) we find a reduction of about 50% in the quasiparticle gap, with much larger reductions in the large $r_s$ limit. As seen in Fig. 1 of Ref. 13, in the small $r_s$ limit, we recover Sondhi’s second-order perturbation theory correction to the spin gap. This correction is a
constant of value 0.58 in effective atomic units. In the dense limit \((r_s \rightarrow 0)\), the second-order perturbation theory is exact.

Smith, MacDonald, and Gumbs\(^{11}\) have performed random phase approximation (RPA) calculations to estimate the effect of Landau-Level mixing. Their results for the parameters of interest in this paper are also plotted on Fig. 1 of Ref. 13. Since RPA tends to underestimate correlations, the fact that the RPA gaps are higher than ours is not surprising.

Skyrmion-Antiskyrmion pair creation energies as computed by Sondhi et al.\(^8\) are also given in Fig. 1 of Ref. 13. The comparison to our present results show that the effect of relaxing the quasiparticle and quasihole states in spin space, i.e., allowing nontrivial spin texture in the states near \(\nu = 1\), has an effect on excitation energies similar in magnitude to that caused by Landau-level mixing. We believe that the character of the excited states of the \(\nu = 1\) systems will be determined by a mixture of both effects.

IV. THE EFFECT OFFINITE THICKNESS

In the actual experimental situation, the electrons at the heterojunction form a quasi-two-dimensional system only in the sense that their motion in the \(z\) direction perpendicular to the interface is restricted to the lowest subband. Even in the lowest subband, the electron wave functions penetrate appreciably into the GaAs layer. Within the triangular-well approximation, the \(z\) extent of the electron wave functions is given by \(\psi(z) = z \exp(-bz/2)\), where \(b = 0.02 - 0.03 \text{ Å}^{-1}\).

In our calculations, we used Ando’s self-consistent calculation for the value of \(b\). In terms of the surface electron density \(N_S\), the depletion layer impurity density \(N_{\text{dep}}\), and the macroscopic dielectric constant of the substrate \(\varepsilon\), \(b\) is given by

\[
b = \left[ \frac{48 \pi m^* e^2 (N_{\text{dep}} + 11N_S/32)}{\varepsilon e^2 h^2} \right]. \tag{33}
\]

While the most rigorous way to take the \(z\) extent into account within our variational formalism would be to propose a three-dimensional many-body wave function for the state of the electron liquid, for computational efficiency we choose instead to introduce an effective interaction between the electrons moving strictly in the \(x\)-\(y\) plane to mimic the effects of their \(z\) extent. Clearly, our effective potential should have the property that (a) it behaves as \(-1/r\) at large distances and (b) it does not have a singularity at zero separation. The latter requirement stems from the observation that, our system being a correlated one, two electrons approaching each other in the \(x\)-\(y\) plane would always avoid each other by getting out of the way perpendicular to the interface.

One solution to the problem of the appropriate effective potential has been introduced by Ando, Fowler, and Stern.\(^{21}\) This method assumes no correlation in the \(z\) direction, and in fact simply averages over the \(z\) extent:

\[
V_{\text{eff}}(r) = \int dz\, dz' \rho(z) \rho(z')/\sqrt{r^2 + (z - z')^2}. \tag{34}
\]

An undesirable feature of the Ando function is that it has a logarithmic singularity for the separation \(r \rightarrow 0\). Instead we use the simpler form \(V_{\text{eff}}(r) = 1/l \sqrt{r^2 + (r - r')^2}\), where \(l\) is the average width of the layer, given by \(3b/2\). Due to the long range of \(V_{\text{eff}}\), we employ a generalized Ewald summation method to evaluate the finite-thickness potential energies of the particles. The formalism is identical to the one used in the evaluation of the Coulomb potential energy, with the new coefficients given in Appendix B.

Figure 3 shows the effect of the finite-thickness parameter \(t\) on the total energy of the \(\nu = 1\) state of a 20-electron simulation cell. For each thickness, we reoptimized the Jastrow factor parameters. We find that the optimal Jastrow parameters can be taken to be the same within our statistical error for thicknesses between \(t = 0\) and \(t = 300 \text{ Å}\), which corresponds to the thicknesses studied for comparison to photoluminescence experiments, discussed below. As the thickness parameter \(t\) increases, the strength of the interactions decreases as \(1/t\) for large \(t\). In particular, the ratio of the typical interaction energy \(V_{\text{eff}}(r_s)\) to the kinetic energy scale of \(\hbar \omega_c\) goes to zero. In the large-\(t\) limit, therefore, the system should behave as if it consisted of noninteracting particles. The energy of the state tends asymptotically to \(\hbar \omega_c/2\) with the difference following a \(1/t\) trend, as expected (Fig. 3).

We obtained the finite-thickness gaps shown in Fig. 4 by using our optimal zero-thickness wave functions and replacing the Coulomb interaction by the finite-thickness potential \(V_{\text{eff}}\) at the \(t\) appropriate to the density of electrons at each of the \(r_s\) values considered. The finite-thickness effect is given by the difference between the curves (b) and (c). We find that the finite-thickness correction (FTC) is nearly 40% at \(r_s = 1\) (\(B \approx 12\) T for GaAs), whereas at \(r_s > 2\) (\(B < 3\) T for GaAs) it is less than 10%.

V. COMPARISON TO PHOTOLUMINESCENCE EXPERIMENTS

Recently photoluminescence experiments\(^2\) have been performed to measure the spin gap of the \(\nu = 1\) quantum Hall liquid in \(\delta\)-doped GaAs heterojunctions. Following Apalkov...
and Rashba\textsuperscript{22} adopt the “sudden approximation” to describe these photoluminescence experiments. Within the sudden approximation, the luminescence photon is assumed to arise from an electron making a transition from the 2D layer to an acceptor state, leaving its exchange-correlation hole behind. In the final state the electron still interacts with the exchange-correlation hole it had left behind. The energy of the photon is then given by the difference in the energy of the electron in the layer and at the impurity. The experiment measures the first moment of the luminescence line $\tilde{h}\tilde{\omega}$. As described by Apalkov and Rashba, for each density of the two-dimensional electron gas (2DEG), $\tilde{h}\tilde{\omega}$ has a cusp as a function of $B$ at $\nu=1$. The strength of the cusp is related to the value of the lowest-energy excitations in the 2DEG. For an ideal zero-thickness 2DEG with no Landau-level mixing, and with the impurity at an infinite distance from the 2DEG, Apalkov and Rashba showed that $\Delta_{SG}=(\nu/2)\delta (\tilde{h}\tilde{\omega}/\nu)$.

We now consider the experimentally realistic case where the impurity is at a finite distance $d$ from the 2DEG and there is Landau-level mixing present. We continue to assume an ideal zero-thickness 2DEG. For a finite system of $N$ particles, or one with periodic boundary conditions,

$$\nu \frac{\delta (\tilde{h}\tilde{\omega})}{\delta \nu} = \frac{N}{2} \frac{\delta (\tilde{h}\tilde{\omega})}{\delta N}. \quad (35)$$

At magnetic field $B$ the photoluminescence line spectral position is given by the energy difference between the initial state and the final state of the particles making the transition. Let the 2DEG be in the $x$-$y$ plane. Assuming a luminescence transition from the origin ($x=0,y=0,z=0$) to the impurity ($x=0,y=0,z=d$), we may write

$$\hbar \omega(B,N) = KE(B,N) + \int d^2r \rho(r)n(r) \left( \frac{e^2}{\epsilon r} - \frac{e^2}{\epsilon \sqrt{d^2+r^2}} \right) + S(B,N). \quad (36)$$

Here $KE(B,N)$ is the kinetic energy of the particle in the 2DEG prior to making the transition, $e$ is its charge, $\epsilon$ is the dielectric constant, $n$ is the density, and $\hbar$ is the pair distribution function as defined in Eq. (32). The two terms in the integral are the interaction energy of the particle with the rest of the particles in the 2DEG at its initial and final position, respectively. $S(B,N)$ is a smooth (cuspless) function of $B$ and $N$, which includes the binding energy of the particle in its final state. Since we are concerned with the cusp in $\hbar \omega$, the smooth part $S(B,N)$ will be omitted from now on.

Denoting the total energy per particle in the 2DEG by $E(B,N)$, we can rewrite Eq. (36):

$$\hbar \omega(B,N) = 2E(B,N) - \int d^2r \rho(r)n(r) \frac{e^2}{\epsilon \sqrt{d^2+r^2}} - KE(B,N). \quad (37)$$

Using Eq. (2) we conclude that the spin gap $\Delta_{SG}$ is related to the photoluminescence line cusp as

$$\Delta_{SG} = \frac{\nu}{2} \frac{\delta (\tilde{h}\tilde{\omega})}{\delta \nu} + \frac{N}{2} \times \left[ \int d^2r \frac{e^2}{\epsilon \sqrt{d^2+r^2}} \delta \frac{\partial}{\partial N} (\tilde{h}(r)n(r)) + \delta \frac{\partial KE(N)}{\partial N} \right]. \quad (38)$$

We refer to the second term on the right-hand side of Eq. (38) as the “finite distance correction” (FDC). It arises from the fact that the electron, having made the transition, still has a finite interaction energy with the exchange-correlation hole it left behind. To evaluate this term, we approximate the 2DEG as a zero-thickness system at the maximum of the lowest subband wave function. In this approximation, the cusp in the interaction of an electron at the impurity with the exchange-correlation hole it left behind in the 2DEG can be evaluated within the same formalism as the finite-thickness effect, with $t$ replaced by $d$.

The third term on the right-hand side of Eq. (38) is the “kinetic energy correction” (KEC). It arises from the fact that the kinetic energy change of the luminescence electron has a cusp at $\nu=1$, due to different amounts of Landau-level mixing in the states below and above $\nu=1$. This term is zero in the lowest-Landau-level approximation.

With our calculated spin gap energy [line (c) in Fig. 4] and the calculated finite distance and kinetic energy corrections, we arrive at a theoretical value for $(\nu/2)\delta (\tilde{h}\tilde{\omega}/\nu)$ which may be compared with experiment. In Fig. 4, the shaded region corresponds to the predicted values of $(\nu/2)\delta (\tilde{h}\tilde{\omega}/\nu)$ with $300 \ A>d>150 \ A$. Since the 2DEG extends into the GaAs layer about 100 $\ A$, these values correspond to $\delta$ doping at $25\sim 40$ nm from the interface. Line (e) in Fig. 4 corresponds to setting $d=180 \ A$. This value produces an excellent fit with the experimental\textsuperscript{2} points.
CONCLUSION

We have described a variational method to calculate the energies of the lowest-energy single spin-flip ($S=1$) excitation in the $\nu=1$ quantum Hall liquid. Our formalism lends itself easily to studying Landau-level mixing effects and the effect of the finite thickness of the experimentally realizable 2DEG. The method gives results consistent with spin gap energies deduced from recent photoluminescence experiments. We have, however, not addressed the issue of higher-spin excitations, such as Skyrmions. We find that, in the systems studied, both Landau-level mixing and finite-thickness effects are very important. It is likely that effects of the same magnitude will be present in the energy of all other types of excitations in the quantum Hall liquids.

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APPENDIX A: CUSP CONDITION

In this appendix we give the details of the calculation of the cusp condition in a magnetic field, using the two relevant interparticle potentials. The case with no magnetic field and the Coulomb interparticle potential is well known. We reproduce here the details of the derivation for completeness.

We solve the interacting two charged particle problem in a magnetic field for small separations. The interacting Hamiltonian is

$$H = \frac{1}{2m*} \sum_i \left( \mathbf{p}_i - \frac{e\mathbf{A}_i}{c} \right)^2 + V(|\mathbf{r}_1 - \mathbf{r}_2|).$$

(A1)

We use the Landau gauge, in which $\mathbf{A} = -B y \hat{x}$, $\mathbf{B} = B \hat{z}$. In relative coordinates, $\mathbf{p} = \left[ (\mathbf{p}_1 - \mathbf{p}_2)/2 \right]$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, and the Hamiltonian that acts on the relative coordinate reads

$$H = K + V(r),$$

(A2)

with

$$K = \frac{\mathbf{p}^2}{2m*} + \frac{eB}{m*} y p_x + \frac{\nu^2 B^2}{4m* c^2} y^2$$

$$- \frac{\hbar^2}{m*} \left( \nabla^2 + i \frac{y}{\hbar} \nabla_x - \frac{y^2}{\hbar^2} \right).$$

(A3)

We assume the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \exp \left( -\frac{y^2 + y_2^2}{2\hbar^2} \right) f(z_1 - z_2) \exp \left[ u(|\mathbf{r}_1 - \mathbf{r}_2|) \right]$$

(A5)

for the solution of the two-particle problem. $f(z)$ here is an arbitrary analytic function of $z$ which vanishes as $z^\nu$ as $z \to 0$. This ansatz, with $u = 0$, would be the most general form of the noninteracting two-particle wave function constrained to the lowest Landau level. $n = 0$ corresponds to the case when the two particles have opposite spin, while $n = 1, 3, 5, \ldots$ corresponds to two particles with the same spin, at Landau-level filling factors $\nu = 1, \frac{1}{3}, \frac{1}{5}, \ldots$. For our study the $n = 0$ and $n = 1$ cases are relevant.

Separating the part of the wave function that depends on the relative coordinate, we can write

$$\Psi(\mathbf{r}) = \exp \left( u(r) - \frac{y^2}{4\hbar^2} \right) f(z).$$

(A6)

The cusp condition can be stated as

$$\lim_{r \to 0} \frac{H \Psi(\mathbf{r})}{\Psi(\mathbf{r})} = E.$$

(A7)

This condition translates into, in terms of $u$,

$$\lim_{r \to 0} \left[ u''(r) + u'(r)^2 + \frac{u'(r)}{r} \right] \left[ 1 + 2 \frac{zf'(r)}{f(r)} + \frac{i y z}{\hbar^2} \right] - \frac{1}{2\hbar^2} \frac{m^*}{\hbar^2} V(r) \right] = \text{const.}$$

(A8)

Here the primes signify derivatives with respect to the argument. We note that the presence of the magnetic field does not affect the form of $u$ in the lowest order. It turns out, therefore, that this derivation remains valid for the no magnetic field case.

In our study, the pseudopotential is chosen to have the general form

$$u(r) = -\frac{A}{\sqrt{r}} \left[ 1 - \exp \left( -Fr^{1/2} - aF^2 r - bF^3 r^{3/2} - cF^4 r^2 \right) \right],$$

(A9)

this form having the desirable $1/\sqrt{r}$ behavior at infinity. By substitution into the cusp condition for $u$, we find that for the case of the Coulomb potential $V(r) = 1/r$ we must set $a = 1/2$, $b = 1/12$, and $c = 0$, while requiring $AF^3/4 = 1/(1 + 2n)$, whereas for the finite-thickness potential $V(r) = (r^2 + d^2)^{-1/2}$ we must set $a = 1/2$, $b = 1/3$, and $c = 1/4$ with no constraint on $A$ and $F$.

APPENDIX B: GENERALIZED EWALD SUMMATION

The goal of an Ewald summation is to find the energy per unit cell of a periodic array of point charges of the same charge and a uniform neutralizing background. Suppose we have, in $D$ dimensions, a periodic system. The lattice vectors which point from the origin of one unit cell to another are $\{\mathbf{R}_j\}$, and the volume of the unit cell is $V$. The reciprocal
lattice vectors \( \{ \mathbf{G}_m \} \) have the property that \( \mathbf{R}_i \cdot \mathbf{G}_m = 2\pi \times (\text{integer}) \) for all \( j \) and \( m \). The particles in each unit cell are located at positions \( \{ \mathbf{r}_i \} \) relative to the unit cell origin. There are \( N_e \) particles per unit cell, so that the density of the compensating background is \( N_e / V \). We assume that the energy of interaction is \( v(\mathbf{r}) = 1 / [f(\mathbf{r})]^z \) for two particles separated by \( \mathbf{r} \).

1. Background derivations

We begin by stating our conventions. Throughout this appendix, integrals without explicit limits have the implicit range of all space. The Fourier transform conventions are

\[
h(\mathbf{q}) = \frac{1}{(2\pi)^D} \int d^D \mathbf{r} e^{i \mathbf{q} \cdot \mathbf{r}}. \quad (B1)
\]

\[
h(\mathbf{r}) = \frac{1}{(2\pi)^D} \int d^D \mathbf{q} e^{-i \mathbf{q} \cdot \mathbf{r}}. \quad (B2)
\]

This is the set of conventions for which the real-space function and its Fourier transform have the same norm.

Our definition of the \( \delta \) function is

\[
\int d^D \mathbf{r} h(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_0) = h(\mathbf{r}_0). \quad (B3)
\]

The Fourier transform of a periodic array of \( \delta \) functions is given by

\[
\frac{1}{(2\pi)^D} \int d^D \mathbf{r} e^{i \mathbf{q} \cdot \mathbf{r}} \sum_{\mathbf{R}} \delta(\mathbf{r} - \mathbf{R}) = \frac{(2\pi)^D}{V} \sum_{\mathbf{G}} \delta(\mathbf{q} - \mathbf{G}). \quad (B4)
\]

where the \( \{ \mathbf{R} \} \) are the lattice vectors defining the periodic array and the \( \{ \mathbf{G} \} \) are the corresponding reciprocal space lattice vectors.

The \( \Gamma \) function is defined as

\[
\Gamma(k) = \int_0^\infty dt t^{k-1} e^{-t}; \quad (B5)
\]

while the complementary incomplete \( \Gamma \) function is

\[
\Gamma(k,z) = \int_z^\infty dt t^{k-1} e^{-t}. \quad (B6)
\]

The Taylor expansion of the complementary incomplete \( \Gamma \) function for small \( z \) is

\[
\Gamma(k,z) = \Gamma(k) - \frac{z^k}{k} + \mathcal{O}(z^{k+1}). \quad (B7)
\]

2. Generalized Ewald summation

The Ewald energy is a sum of three terms:

\[
E_{\text{Ewald}} = E_{b \rightarrow b} + E_{e \rightarrow b} + E_{e \rightarrow e}. \quad (B8)
\]

\( E_{b \rightarrow b} \) is the energy of interaction of the background charge in one unit cell with the background charge in all space:

\[
E_{b \rightarrow b} = \frac{e^2 N_e}{2V} \int_{\text{one cell}} d^D \mathbf{r} \int d^D \mathbf{r}' \frac{1}{f(\mathbf{r} - \mathbf{r}')^2} \quad (B9)
\]

\[
= \frac{e^2 N_e^2}{2V} \int d^D \mathbf{r} \frac{1}{f(\mathbf{r})^2}. \quad (B10)
\]

\( E_{e \rightarrow b} \) is the energy of interaction of the point charges in one unit cell with the oppositely charged background charge in all space:

\[
E_{e \rightarrow b} = \frac{e^2 N_e^2}{2V} \int_{\text{one cell}} d^D \mathbf{r} \frac{1}{f(\mathbf{r})^2}. \quad (B11)
\]

\( E_{e \rightarrow e} \) is the energy of interaction of the point charges in one unit cell with the point charges in all space:

\[
E_{e \rightarrow e} = \frac{e^2}{2} \sum_{\mathbf{R} \mathbf{R}'} \frac{1}{f(\mathbf{R} + \mathbf{R}' - \mathbf{r})^2}. \quad (B12)
\]

The prime over the summation means that we avoid the self-interaction terms, i.e., the ones where both \( i = j \) and \( \mathbf{R} = 0 \). We do, however, include the interaction of a particle with its own images in other cells.

We now recast the expression for the Ewald sum into a form that will prove useful later. First, we rewrite the interaction using the definition of the \( \Gamma \) function. We make the substitution \( t = f(\mathbf{r}) u \) into Eq. (B5):

\[
\Gamma(k) = f(\mathbf{r})^k \int_0^\infty du u^{k-1} e^{-f(\mathbf{r}) u}. \quad (B13)
\]

This gives us an obscure but useful way to rewrite the interaction:

\[
\frac{1}{f(\mathbf{r})^k} = \frac{1}{\Gamma(k)} \int_0^\infty du u^{k-1} e^{-f(\mathbf{r}) u}. \quad (B14)
\]

We can now separate the \( E_{e \rightarrow e} \) summation into two parts by doing the above integral from 0 to \( \alpha \) and from \( \alpha \) to \( \infty \):

\[
E_{e \rightarrow e} = \frac{e^2}{2\Gamma(k)} \sum_{\mathbf{R}} \left[ \int_0^\alpha du u^{k-1} e^{-f(\mathbf{r} + \mathbf{R} - \mathbf{r}_i) u} \right. \\
\left. + \int_\alpha^\infty du u^{k-1} e^{-f(\mathbf{r} + \mathbf{R} - \mathbf{r}_i) u} \right] = E_1 + E_2. \quad (B15)
\]

The parameter \( \alpha \) is completely arbitrary. However, as we will see, it governs the relative rate of convergence of \( E_1 \) and \( E_2 \).

We evaluate \( E_1 \) in Fourier space. We then define a function \( g(\mathbf{r}) \) which generalizes the sum found in \( E_1 \) by introducing a position variable \( \mathbf{r} \):

\[
g(\mathbf{r}) = \sum_{\mathbf{R}} e^{-f(\mathbf{r} + \mathbf{R} - \mathbf{r}_i) u}. \quad (B16)
\]
Note that \( g(\mathbf{r}) \) includes the self-interaction terms. Performing the Fourier transform, we obtain
\[
g(\mathbf{q}) = \frac{1}{(2\pi)^D} \int d^D \mathbf{r} \sum_{\mathbf{R}} e^{-f(\mathbf{r}+\mathbf{R})} e^{i\mathbf{q} \cdot \mathbf{r}}.
\]
(B17)

We may simplify this by substituting \( t = \mathbf{r} + \mathbf{r}_j + \mathbf{R} - \mathbf{r}_i \):
\[
g(\mathbf{q}) = \frac{1}{(2\pi)^D} \sum_{\mathbf{R}} \int d^D t e^{-f(t)} e^{i\mathbf{q} \cdot t} e^{-i\mathbf{q} \cdot (\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i)}
\]
\[
= F_u(\mathbf{q}) \sum_{\mathbf{r}_j, \mathbf{r}_i} e^{-i\mathbf{q} \cdot (\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i)}.
\]
(B18)

The last equality uses the following definition:
\[
F_u(\mathbf{q}) = \frac{1}{(2\pi)^D} \int d^D \mathbf{r} e^{-f(\mathbf{r})} e^{i\mathbf{q} \cdot \mathbf{r}}.
\]
(B19)

The sum in Eq. (B18) using Eq. (B4) reduces to
\[
\sum_{j=1}^{N_e} e^{i\mathbf{q} \cdot \mathbf{r}_j} \sum_{j=1}^{N_e} e^{-i\mathbf{q} \cdot \mathbf{r}_j} \sum_{\mathbf{R}} e^{-i\mathbf{q} \cdot \mathbf{R}} = \sum_{\mathbf{G}} \rho^*_G \rho_G \delta(\mathbf{q} - \mathbf{G}),
\]
where
\[
\rho_G = \frac{(2\pi)^D}{V} \sum_{j=1}^{N_e} e^{i\mathbf{G} \cdot \mathbf{r}_j}.
\]
(B21)

The sum in \( E_1 \) corresponds to \( g(\mathbf{r} = 0) \):
\[
g(\mathbf{r} = 0) = \frac{V}{(2\pi)^D} \sum_{\mathbf{G}} \rho^*_G \rho_G F_u(\mathbf{G}),
\]
(B22)

\[E_1 = \frac{e^2}{2 V} \int_0^\infty du u e^{-f(\mathbf{r} = 0)u} \]
\[+ \frac{V}{(2\pi)^D} \sum_{\mathbf{G}} \rho^*_G \rho_G F_u(\mathbf{G}), \]
(B23)

The first term in brackets subtracts off the self-interaction terms which were included in \( g(\mathbf{r}) \). We define \( h(\mathbf{G}) \) and \( H \):
\[
h(\mathbf{G}) = \frac{V}{(2\pi)^D} \int_0^\infty du u e^{-f(\mathbf{r} = 0)u} \]
\[+ \frac{V}{(2\pi)^D} \sum_{\mathbf{G}} \rho^*_G \rho_G F_u(\mathbf{G}), \]
(B24)

\[H = \frac{N_e}{\Gamma(k)} \int_0^\infty du u e^{-f(\mathbf{r} = 0)u} \]
(B25)

With these definitions,
\[
E_1 = \frac{e^2}{2} \left[ -H + \sum_{\mathbf{G}} \rho^*_G \rho_G h(\mathbf{G}) \right].
\]
(B26)

We turn our attention to \( E_2 \), which is evaluated in real space. With the change of variables \( u = t / f(\mathbf{r}) \) we can rewrite the integrals appearing in the expression for \( E_2 \) in Eq. (B15):
\[
\int_\alpha^\infty du u^{k-1} e^{-f(\mathbf{r})u} = \frac{1}{f(\mathbf{r})} \int_0^\infty dt t^{k-1} e^{-t} \]
\[= \frac{1}{f(\mathbf{r})^k} \Gamma(k, af(\mathbf{r})). \]
(B27)

Defining
\[
w(r) = \frac{\Gamma(k, af(\mathbf{r}))}{f(\mathbf{r})^k \Gamma(k)}
\]
permits a rewriting of \( E_2 \):
\[
E_2 = \frac{e^2}{2} \sum_{\mathbf{r}_j, \mathbf{r}_i} w(\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i).
\]
(B29)

Adding \( E_{b-b} \), \( E_{e-b} \), \( E_1 \), and \( E_2 \), we get the full Ewald energy:
\[
E_{\text{Ewald}} = -\frac{e^2 N_e^2}{2V} \int d^{D}r \frac{1}{f(\mathbf{r})^k} + \frac{e^2}{2} \left[ -H + \sum_{\mathbf{G}} \rho^*_G \rho_G h(\mathbf{G}) \right] \]
\[+ \frac{e^2}{2} \sum_{\mathbf{r}_j, \mathbf{r}_i} w(\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i). \]
(B30)

At this point, we may simplify the above expression by subsuming the background terms into the \( h(\mathbf{G} = 0) \). Indeed, the \( \mathbf{G} = 0 \) term of \( E_1 \) and the background term \( E_{e-b} + E_{b-b} \) have similar forms:
\[
\frac{e^2}{2} \rho^*_G \rho_G h(\mathbf{G} = 0) = \frac{e^2 N_e^2}{2 V \Gamma(k)} \int_0^\alpha du u^{k-1} \int d^{D}r e^{-f(\mathbf{r})u} \]
(B31)

and
\[
E_{e-b} + E_{b-b} = -\frac{e^2 N_e^2}{2 V \Gamma(k)} \int_0^\infty du u^{k-1} \int d^{D}r e^{-f(\mathbf{r})u}. \]
(B32)

Therefore, combining the \( \mathbf{G} = 0 \) term of \( E_1 \) and the background yields
\[
-\frac{e^2 N_e^2}{2 V \Gamma(k)} \int_0^\infty du u^{k-1} \int d^{D}r e^{-f(\mathbf{r})u}. \]
(B33)

As a result, it is convenient to redefine \( h(\mathbf{G} = 0) \) to incorporate the background terms:
\[
h(\mathbf{G} = 0) = -\frac{V}{(2\pi)^D} \int_0^\infty du u^{k-1} F_u(\mathbf{G} = 0).
\]
(B34)

With this new definition,
\[
E_{\text{Ewald}} = \frac{e^2}{2} \left[ -H + \sum_{\mathbf{G}} \rho^*_G \rho_G h(\mathbf{G}) \right] + \frac{e^2}{2} \sum_{\mathbf{r}_j, \mathbf{r}_i} w(\mathbf{r}_j + \mathbf{R} - \mathbf{r}_i). \]
(B35)

Note that all the sums involve short-ranged functions only, so a small number of terms should suffice in their numerical evaluation.
3. Power law and Coulomb interaction

We now turn to the evaluation of $h(G)$ and $H$ for specific cases. For the case of a power law, $v(r) = 1/r^{n}$ (a special case of which is the Coulomb interaction), the interaction can be described using $f(r) = r^{2}$ and $k = n/2$. $F_{u}(G)$ for this case is given by

$$F_{u}(G) = \frac{1}{(2\pi)^{D/2}}e^{-G^{2}/4u}. \quad (B36)$$

Hence $h(G \neq 0)$ is

$$h(G) = \frac{V}{(4\pi)^{D/2}\Gamma(n/2)} \int_{0}^{a} du u^{n/2-1-D/2}e^{-G^{2}/4u}, \quad (B37)$$

which can be further simplified through the change of variables $t = G^{2}/4u$:

$$h(G) = \frac{(G/2)^{n-D}V}{(4\pi)^{D/2}\Gamma(n/2)} \int_{0}^{\infty} dt t^{D-n-1}e^{-t}$$

$$= \frac{2^{D-n}V\Gamma\left(D-n,\frac{G^{2}}{2} \right)}{G^{D-n}(4\pi)^{D/2}\Gamma(n/2)}.$$ 

For $G = 0$

$$h(G = 0) = -\frac{V}{(4\pi)^{D/2}\Gamma(n/2)} \int_{a}^{\infty} du u^{n/2-1-D/2}$$

$$= -\frac{2V}{(4\pi)^{D/2}\Gamma(n/2)} \frac{\Gamma\left(D-n,\frac{G^{2}}{2} \right)}{\Gamma(D-n)}. \quad (B39)$$

The $H$ term is given by

$$H = \frac{N_{e}}{\Gamma(n/2)} \int_{0}^{a} du u^{n/2-1}e^{-a^{2}u}$$

$$= \frac{N_{e}}{\Gamma(n/2)} \left[\frac{\Gamma(n/2)}{\Gamma(n/2,d^{2})} \right]. \quad (B40)$$

With these expressions for $H$ and $h(G)$, the entire Ewald energy can be computed. As mentioned above, the value of the Ewald sum is independent of the parameter $\alpha$. However, the real space and the reciprocal space sums converge in a comparable number of terms if $\alpha$ satisfies

$$\alpha R_{\text{max}}^{2} = G_{\text{max}}^{2}/4\alpha.$$ 

4. Finite-thickness interactions

For the case of our model finite-thickness interaction, $v(r) = 1/(r^{2}+d^{2})^{n/2}$, we may choose $f(r) = r^{2}+d^{2}$ and $k = n/2$. In this case we have

$$F_{u}(G) = \frac{1}{(2\pi)^{D/2}}e^{-d^{2}u-G^{2}/4u}. \quad (B41)$$

Hence $h(G)$ can be written as

$$h(G) = \frac{V}{(4\pi)^{D/2}\Gamma(n/2)} \int_{0}^{a} du u^{n/2-1-D/2}e^{-d^{2}u-G^{2}/4u}.$$ 

While the $G \neq 0$ integral must be done numerically and tabulated, for $G = 0$ the integral can be done analytically:

$$h(G = 0) = -\frac{V}{(4\pi)^{D/2}\Gamma(n/2)} \int_{a}^{\infty} du u^{n/2-1-D/2}e^{-d^{2}u}$$

$$= -\frac{Vd^{D-n}}{(4\pi)^{D/2}\Gamma(n/2)} \frac{\Gamma\left(D-n,\frac{d^{2}}{2} \right)}{\Gamma(D-n)}. \quad (B43)$$

The $H$ term is given by

$$H = \frac{N_{e}}{\Gamma(n/2)} \int_{0}^{a} du u^{n/2-1}e^{-d^{2}u}$$

$$= \frac{N_{e}}{\Gamma(n/2)} \left[\frac{\Gamma(n/2)}{\Gamma(n/2,d^{2})} \right]. \quad (B44)$$

With these definitions for $H$ and $h(G)$, the entire Ewald energy can be computed. The parameter $\alpha$ is chosen similarly to the Coulombic case.

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2I. V. Kukushkin et al., Europhys. Lett. 22, 287 (1993); and (private communication).


