Trial wave functions, molecular states, and ro-vibrational spectra in the lowest Landau level: A universal description for bosons and fermions

Constantine Yannouleas and Uzi Landman

School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430

Through the introduction of a class of appropriate translationally invariant trial wave functions, we show that the strong correlations in the lowest Landau level (LLL) reflect in finite systems the emergence of intrinsic point-group symmetries associated with rotations and vibrations of molecules formed through particle localization. This molecular description is universal, being valid for both bosons and fermions, for both the yrast and excited states of the LLL spectra, and for both low and high angular momenta. This physical picture is fundamentally different from the "quantum-fluid" one associated with Jastrow-type trial functions.

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Motivation. — Following the discovery [1] of the fractional quantum Hall effect (FQHE) in two-dimensional (2D) semiconductor heterostructures under high magnetic fields (B), the description of strongly correlated electrons in the lowest Landau level (LLL) developed into a major branch of theoretical condensed matter physics [2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. Early on, it was realized that the essential many-body physics in the LLL could be captured through trial wave functions. Prominent examples are the Jastrow-type Laughlin [2], composite fermion [6], and Moore and Read’s Pfaffian functions, representing quantum-liquid states [2]. More recently, the field of semiconductor quantum dots [14] helped to focus attention on finite systems with a small number (N) of electrons. Theoretical investigations of such finite systems led to the introduction of "crystalline"-type LLL trial functions referred to as rotating electron molecules (REMs) [12, 14].

Most significantly, the burgeoning field of trapped ultracold neutral gases has generated recently an unparalleled interest regarding the fundamental aspects (including the appropriateness of trial functions) of strongly correlated states in the lowest Landau level [17, 18, 19, 20, 21, 22, 23, 24, 25, 26]; in this case, the LLL manifold of degenerate single-particle orbitals arises as a result of the rapid rotation (with rotational frequency Ω) of the trap. Furthermore, it is anticipated that small assemblies of ultracold bosonic atoms will become technically available in the near future [27] and that they will provide an excellent vehicle [22, 24, 26, 27] for experimentally reaching exotic physical behavior beyond the mean-field Gross-Pitaevskii regime and for testing the rich variety of proposed LLL trial wave functions.

A universal description of the full LLL spectra (including both yrast [28] and all excited states), however, is still missing. To remedy this, a unified theory for the LLL spectra of a small number of particles valid for both statistics (i.e., for both bosons and fermions) is introduced in this paper. The LLL spectra are shown to be associated with fully quantal ro-vibrational molecular (RVM) states, i.e., states described by trial wave functions akin to the REM functions of Ref. [12]. It is remarkable that the numerical results of the present theory agree within machine precision with exact-diagonalization (EXD) results, including energies, wave functions, and overlaps. This behavior outperforms the behavior of all other trial functions, including those of the composite-fermion view [17, 16, 29]. The RVM functions and corresponding point-group symmetries express the emergent many-body intrinsic structure of the highly correlated LLL states.

Theory. — The RVM functions have the general form (within a normalization constant):

\[ \Phi^{\text{RXM}}_{\mathcal{L}}(n_1, n_2)Q^m_{\lambda}|0> , \]

where \((n_1, n_2)\) indicates the molecular configuration (here we consider two concentric rings) of point-like particles with \(n_1\) \((n_2)\) particles in the first (second) ring. The particles on each ring form regular polygons. The index RXM stands for either REM, i.e., a rotating electron molecule, or RBM, i.e., a rotating boson molecule. \(\Phi^{\text{RXM}}_{\mathcal{L}}(n_1, n_2)\) alone describes pure molecular rotations associated with magic angular momenta \(\mathcal{L} = \mathcal{L}_0 + n_1k_1 + n_2k_2\), with \(k_1, k_2\) being nonnegative integers; \(\mathcal{L}_0 = N(N - 1)/2\) for electrons and \(\mathcal{L}_0 = 0\) for bosons. The product in Eq. (1) combines rotations with vibrational excitations, the latter being denoted by \(Q^m_{\lambda}\), with \(\lambda\) being an angular momentum; the superscript denotes raising to a power \(m\). Both \(\Phi^{\text{RXM}}_{\mathcal{L}}\) and \(Q^m_{\lambda}\) are homogeneous polynomials of the complex particle coordinates \(z_1, z_2, \ldots, z_N\), of order \(\mathcal{L}\) and \(\lambda m\), respectively. The total angular momentum \(L = \mathcal{L} + \lambda m\). \(Q^m_{\lambda}\) is always symmetric in these variables; \(\Phi^{\text{RXM}}_{\mathcal{L}}\) is antisymmetric (symmetric) for fermions (bosons). \(|0> = \prod_{i=1}^{N} \exp[-z_i z_i^*/2]\); this product of Gaussians will be omitted henceforth.

The analytic expressions for the \(\Phi^{\text{REM}}_{\mathcal{L}}\) (for fully polarized electrons) were derived in Ref. [12] employing a two-step method: (i) First a single Slater determinant [that breaks the rotational (circular) symmetry] was constructed using displaced Gaussians as electronic orbitals,
expression for both bosons and electrons, namely, by the terms appearing in Eq. (4).

The phase factor is due to the gauge invariance. \( z \equiv x - iy \), and all lengths are in dimensionless units of \( l_B \sqrt{2} \), with the magnetic length \( l_B = \sqrt{\hbar/(m_e \omega_c)} \); \( \omega_c = eB/(m_e c) \) is the cyclotron frequency. The centers \( Z_j \equiv Y_j + iX_j \), \( j = 1, 2, \ldots, N \) of the Gaussians are the vertices of the regular polygons in the \((n_1, n_2)\) geometric arrangement. (ii) A subsequent step of symmetry restoration was performed using the projection operator \( P(L) = \frac{1}{2\pi} \int_0^{2\pi} d\gamma e^{i\gamma(L-L')} \), where \( L = \sum_{i=1}^N \hat{L}_i \) is the total angular momentum operator; this yielded trial wave functions with good total angular momenta \( L \) \([12, 14]\).

Analytic expressions for the \( \Phi_{L}^{\text{RBM}} \) (for spinless bosons) can also be derived using the two-step method. Naturally, in the first step one constructs a permanent out of the orbitals of Eq. (2); one also uses the equivalence \( \omega_c \rightarrow 2\Omega \) between the cyclotron frequency (electrons) and the rotational frequency (bosons) \([14]\). The expressions for any number \( N \) of bosons and any molecular configuration \((n_1, n_2, \ldots, n_q)\) will be presented in Ref. \([30]\). Here we present as an illustrative example the simpler case of \( N = 3 \) bosons having a \((0, 3)\) one-ring molecular configuration. One has (within a normalization constant)

\[
\Phi_{L}^{\text{RBM}}(0, 3) = \sum_{0 \leq l_1 \leq l_2 \leq l_3} C(l_1, l_2, l_3) \text{Perm}[z_{1,1}' \ldots z_{3,1}'],
\]

(3)

where the symbol "Perm" denotes a permanent with elements \( z_{i,j}' \), \( i, j = 1, 2, 3 \); only the diagonal elements are shown in Eq. (3). The coefficients were found to be:

\[
C(l_1, l_2, l_3) = \left( \prod_{i=1}^3 l_i! \right)^{-1} \left( \prod_{k=1}^M p_k! \right)^{-1} \times \left( \sum_{1 \leq i < j \leq 3} \cos \left[ \frac{2\pi(l_i - l_j)}{3} \right] \right),
\]

(4)

where \( 1 \leq M \leq 3 \) denotes the number of different indices in the triad \((l_1, l_2, l_3)\) and the \( p_k \)'s are the multiplicities of each one of the different indices. For example, for \((1, 1, 4)\), one has \( M = 2 \) and \( p_1 = 2, p_2 = 1 \).

The \( \Phi_{L}^{\text{REM}} \) expressions for electrons in a \((0, N)\) or a \((1, N)\) configuration are given by Eqs. (2) and (4) of Ref. \([13]\), respectively. For electrons \((1)\) \( M = N \) in all instances and (2) a product of \textit{sin} terms replaces the \textit{sum of cosine} terms appearing in Eq. (4).

We note that \( \Phi_{L}^{\text{REM}}(n_1, n_2) = 0 \) for both bosons and electrons when \( L \neq L_0 + n_1k_1 + n_2k_2 \). This selection rule follows directly from the point group symmetries of the \((n_1, n_2)\) molecular configurations.

The vibrational excitations \( Q_{\lambda} \) are given by the same expression for both bosons and electrons, namely, by the symmetric polynomials:

\[
Q_{\lambda} = \sum_{i=1}^{N} (z_i - z_c)^\lambda,
\]

(5)

where \( z_c = (1/N) \sum_{i=1}^{N} z_i \) is the coordinate of the center of mass and \( \lambda > 1 \) is a prime number. Vibrational excitations of a similar form, i.e., \( Q_{\lambda} = \sum_{i=1}^{N} z_i^\lambda \) (and certain other variations), have been used earlier to approximate \textit{part} of the LLL spectra. Such earlier endeavors provided valuable insights, but overall they remained inconclusive; for electrons over the maximum density droplet (with magic \( L = L_0 \)), see Refs. \([8, 9]\); and for electrons over the \( \nu = 1/3 (\nu = L_0/L) \) Jastrow-Laughlin trial function (with magic \( L = 3L_0 \)), see Ref. \([10]\); and for bosons in the range \( 0 \leq L \leq N \), see Refs. \([17, 20, 21]\).

The advantage of expression \([31]\) is that it is translationally invariant (TI), a property also shared by both the \( \Phi_{L}^{\text{RBM}} \) and \( \Phi_{L}^{\text{REM}} \) trial functions. In the following, we will discuss illustrative cases, which will demonstrate that the molecular trial functions of Eq. \([11]\) provide a correlated basis that spans the TI subspace \([6, 24, 32]\) of nonspurious states in the LLL spectra. The dimension \( D_{\text{TI}}(L) \) of the TI subspace is much smaller than the dimension \( D_{\text{EXD}}(L) \) of the exact-diagonalization (EXD) space spanned by the uncorrelated determinants \( \text{Det}[z_{1,1}' \ldots z_{N,1}'] \) or permanents \( \text{Perm}[z_{1,1}' \ldots z_{N,1}'] \). The remaining \( D_{\text{EXD}}(L) - D_{\text{TI}}(L) \) states are \textit{spurious} center-of-mass excitations (generated by applying \( Q_{\lambda}^{\ell} \)) whose energies coincide with those appearing at all the other smaller angular momenta \([3]\). Thus \( D_{\text{TI}}(L) = D_{\text{EXD}}(L) - D_{\text{EXD}}(L - 1) \); see Tables \([4, 11]\).

\textbf{Three spinless bosons} — Only the \((0, 3)\) molecular configuration and the dipolar \( \lambda = 2 \) vibrations are at play (as checked numerically), i.e., the full TI spectra at any \( L \) are spanned by the wave functions

\[
\Phi_{3k}^{\text{RBM}}(0, 3)Q_{2}^m \Rightarrow \{k, m\},
\]

(6)

where \( k = m = 0, 1, 2, \ldots, \) and \( L = 3k + 2m; \) these states are always orthogonal. This represents a remarkable analogy with the case of \( N = 3 \) electrons (see below).

Table \([4]\) provides the systematics of the molecular description for the beginning \((0 \leq L \leq 12)\) of the LLL spectrum. There are several cases when the TI subspace has dimension one and the exact solution coincides with a single \( \{k, m\} \) state. For \( L = 0 \) the exact solution coincides with \( \Phi_0^{\text{RBM}} = 1 (Q_{0}^{0} = 1) \); this is the only case when an LLL state has a Gross-Pitaevskii form, i.e., it is a single permanent \([0]\) in Eq. \([11]\). For \( L = 2 \), we found \( \Phi_2^{\text{exact}} \propto Q_2 \) (for the subscript \([i]\), see caption of Table \([1]\)), and since \([\text{see Eq. } 3]\) \( Q_2 \propto (z_1 - z_c)(z_2 - z_c) + (z_1 - z_c)(z_3 - z_c) + (z_2 - z_c)(z_3 - z_c) \), this result agrees with the findings of Refs. \([20, 24]\) concerning ground states of the range \( 0 \leq L \leq N \). For \( L = 3 \), one finds
TABLE I: Spectra of three spinless bosons. Second column: Dimensions of the EXD and the nonspurious TI (in parenthesis) spaces. Fourth to sixth columns: Matrix elements [in units of $g/(\pi\Lambda^2)$, $\Lambda = \sqrt{\hbar/(m\Omega)}$] of the repulsive contact interaction $g\delta(z_i - z_j)$ between the nonspurious states $\{k, m\}$ [see Eq. (3)]. The total angular momentum $L = 3k + 2m$. Last three columns: Total energy eigenvalues from the diagonalization of the associated matrix of dimension $D^{\text{TI}}(L)$. There is no nonspurious state with $L = 1$. The full spectrum at a given $L$ is constructed by including, in addition to the listed TI total-energy eigenvalues $[D^{\text{TI}}(L)$ in number], all the energies associated with angular momenta smaller than $L$. An integer in square brackets indicates the energy ordering in the full spectrum, with [1] denoting a yrast state. Seven decimal digits are displayed, but the total energies agree with the EXD ones within machine precision.

| $L$ | $D^{\text{EXD}}(D^{\text{TI}})$, $(k, m)$ | Matrix elements | Total energy eigenvalues (TI) |
|-----|------------------------------------------|----------------|--------------------------------|
| 0   | $\{0, 0\}$                              | 1.5000000      | 1.5000000                     |
| 1   | $\{0, 1\}$                              | 0.7500000      | 0.7500000                     |
| 2   | $\{1, 0\}$                              | 0.3750000      | 0.3750000                     |
| 3   | $\{1, 2\}$                              | 0.5625000      | 0.5625000                     |
| 4   | $\{2, 0\}$                              | 0.4687500      | 0.4687500                     |
| 5   | $\{1, 1\}$                              | 0.1482318      | 0.1482318                     |
| 6   | $\{2, 1\}$                              | 0.0468750      | 0.0468750                     |
| 7   | $\{1, 2\}$                              | 0.3750000      | 0.3750000                     |
| 8   | $\{2, 2\}$                              | 0.1960922      | 0.1960922                     |
| 9   | $\{1, 3\}$                              | 0.5002441      | 0.5002441                     |

$\Phi_{\text{REM}}$ and $\Phi_3$ differ. Since $\Phi_3 \propto (z_1 - z_2) (z_2 - z_3) (z_3 - z_4)$ [see Eq. (3)], this result agrees again with the findings of Refs. [20, 34]. For $L = 5$, the single nonspurious state is an excited one, $\Phi_{\text{REM}} \propto \Phi_3 Q_2$. For $L = 6$, the ground-state is found to be $\Phi_{\text{REM}} \propto -16\Phi_9^{\text{RBM}}/9 + Q_2^4/4 = (z_1 - z_2)^2 (z_2 - z_3)^2 (z_3 - z_4)^2$, i.e., the bosonic Laughlin function is $\nu = 1/2$ equivalent to an RBM state that incorporates vibrational correlations. For $L \geq N(N - 1)$ (i.e., $\nu \leq 1/2$), the EXD yrast energies equal zero, and with increasing $L$ the degeneracy of the zero-energy states for a given $L$ increases. It is important that this nontrivial behavior is reproduced faithfully by the present method (see Table I).

Three electrons — Although unrecognized, the solution of the problem of three spin-polarized electrons in the LLL using molecular trial functions has been presented in Ref. [33]. Indeed, the wave functions in Jacobi coordinates in Eq. (18) of Ref. [33] are precisely of the form $\Phi^{\text{RBM}}_{2k} Q_{2}^m$, as can be checked after transforming back to cartesian coordinates [36]. It is noteworthy that Laughlin did not present molecular trial functions for electrons with $N > 3$, or for bosons for any $N$. This is done in the present paper. We further note that the well-known Jastrow-Laughlin ansatz $\prod_{1 \leq i < j \leq N} (z_i - z_j)^{2\nu+1}$ introduced in Ref. [2] is described as a quantum-fluid state [2]. The quantum-liquid-picture interpretation of this ansatz is inconsistent with the RVM functions of Eq. (11).

Four electrons — For $N = 4$ spin-polarized electrons, one needs to consider rovibrational states [see Eq. (11)] for two distinct molecular configurations, i.e., $\Phi^{\text{REM}}_{6+4k} Q_{2}^m$ and $\Phi^{\text{REM}}_{6+3k}(1, 3) Q_2^m$. Vibrational excitations with $\lambda \geq 2$ must also be considered. In this case the molecular basis states are not always orthogonal, and the Gram-Schmidt orthogonalization is implemented. Table II summarizes the molecular description in the start of the LLL spectrum ($6 \leq L \leq 15$ and $L = 18$).

We note that in several cases the nonspurious states are given by a single trial state as defined in Eq. (11). Indeed for $L = 9$ the yrast state is a pure REM state, i.e., $\Phi_{\text{REM}}(1, 3)$. For $L = 11$ the single nonspurious state is the first excited state in the full spectrum, coinciding with the molecular vibration $\Phi_{\text{REM}}(1, 3) Q_2^2$.

Of particular interest is the $L = 18$ case; it corresponds to the celebrated $\nu = 1/3$ fractional filling, which is considered [2] as the prototype of quantum liquid states. However, in this case we found (see Table II) that the exact nonspurious solutions are linear superpositions of seven molecular states involving dipole ($\lambda = 2$) and octupole ($\lambda = 3$) vibrations over both the (0,4) and (1,3) configurations. Focusing on the yrast state with $L = 18$, we found that its largest component is the pure $\Phi_{\text{REM}}(0, 4) Q_2^2$ with a 0.9294 overlap with the EXD solution; the contributions of the remaining six states are much smaller, but they bring the overlap to precisely unity. Unlike the $\nu = 1/2$ case of bosons, we stress that the fermionic Jastrow-Laughlin functions at all $\nu$’s exhibit less-than-unity overlaps [2, 11].

Of great interest also is the $L = 30$ ($\nu = 1/5$) case, which in the composite-fermion picture was found to be susceptible to a competition between crystalline and liquid orders. However, we found that the exact nonspurious states for $L = 30$ are actually linear superpositions of the following $19 = D^{\text{TI}}(L = 30)$ RVM functions: $\Phi_{6+4k}^{\text{REM}}(0, 4) Q_{2}^{2k}$, with $k = 0, 1, 2, 3, 4$. |
interaction in the above TI subspace yielded an en-
centric polygonal-ring configurations. We stress, particu-
tions of molecules of localized particles arranged in con-

group symmetries associated with rotations and vibra-
reflects the spontaneous emergence of intrinsic point-

nature of strong correlations in the lowest Landau level
linear superpositions of these trial functions. Thus the
by the rovibrational molecular trial functions introduced
and for both low and high angular momenta) is spanned
spectra of small systems (whether fermions or bosons,
(based on Laughlin, composite-fermion, and Pfaffian
functions) have been assumed [2, 11, 26] to apply.

TABLE II: Spectra of four spin-polarized electrons. Second column: Dimensions of the EXD and the nonspurious TI (in parenthesis) spaces. Last three columns: Total energy eigenvalues [in units of $e^2/(\kappa l_B)$] from the diagonalization of the Coulomb interaction $e^2/(\kappa r_{ij})$ in the TI subspace spanned by the trial functions $\Phi_{REM}^{6+4k}(0, 4)Q_2^\lambda$ and $\Phi_{REM}^{6+3k}(1, 3)Q_2^\lambda$. Third to sixth columns: the molecular configurations $(n_1, n_2)$ and the quantum numbers $k, \lambda$ and $m$ are indicated within brackets. There is no nonspurious state with $L = 7$. An integer in square brackets indicates the energy ordering of each nonspurious state in the full spectrum, obtained by considering the spurious center-of-mass excitations (see also caption of Table I). Eight
decimal digits are displayed, but the total energies agree with the corresponding EXD results within machine precision.

| $L$ | $D^{EXD}$ ($D^{TI}$) | $(n_1, n_2)(k, \lambda, m)$ | Total energy eigenvalues (TI) |
|-----|---------------------|--------------------------|-------------------------------|
| 6   | 1(1)               | (0,4)(0,1,0)              | 2.22729079[1]                |
| 8   | 2(1)               | (0,4)(0,2,1)              | 2.09240211[1]                |
| 9   | 3(1)               | (1,3)(1,1,0)              | 1.93480798[1]                |
| 10  | 5(2)               | (0,4)(1,1,0)              | (0,4)(0,2,2)                 | 1.78508849[1] 1.97809256[3] |
| 11  | 6(1)               | (1,3)(1,2,1)              | 1.86157215[2]                |
| 12  | 9(3)               | (0,4)(1,2,1)              | (0,4)(1,2,3) (1,3)(2,2,0)    | 1.68518201[1] 1.76757420[2] 1.88068652[5] |
| 13  | 11(2)              | (1,3)(1,2,2)              | (0,4)(1,3,1)                 | 1.64156849[1] 1.79962234[5] |
| 14  | 15(4)              | (0,4)(2,2,0)              | (0,4)(1,2,2) (0,4)(1,2,4)    | 1.50065835[1] 1.63524962[2] 1.72910626[5] |
| 15  | 18(3)              | (1,3)(3,2,0)              | (1,3)(2,3,1) (1,3)(1,3,2)    | 1.52704695[2] 1.62342533[3] 1.74810279[8] |
| 18  | 34(7)              | (0,4)(3,2,0)              | (0,4)(2,2,2) (0,4)(1,2,4)    | 1.30572905[1] 1.41507954[2] 1.43427543[4] |

Conclusions. — The many-body Hilbert space corresponding to the translationally invariant part of the LLL spectra of small systems (whether fermions or bosons, and for both low and high angular momenta) is spanned by the rovibrational molecular trial functions introduced in Eq. (1). The yrast and excited states for both short- and long-range interactions can always be expressed as linear superpositions of these trial functions. Thus the nature of strong correlations in the lowest Landau level reflects the spontaneous emergence of intrinsic point-group symmetries associated with rotations and vibrations of molecules of localized particles arranged in concentric polygonal-ring configurations. We stress, particularly, the validity and numerical superiority of the present molecular theory for low angular momenta, where fundamentally different “quantum-liquid” physical pictures (based on Laughlin, composite-fermion, and Pfaffian
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