Microscopic analytical theory of a correlated, two-dimensional

$N$-electron gas in a magnetic field

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Abstract

We present a microscopic, analytical theory describing a confined $N$-electron gas in two dimensions subject to an external magnetic field. The number of electrons $N$ and strength of the electron-electron interaction can be arbitrarily large, and all Landau levels are included implicitly. For any value of the magnetic field $B$, the correlated $N$-electron states are determined by the solution to a universal effective problem which resembles a ficticious particle moving in a multidimensional space, without a magnetic field, occupied by potential minima corresponding to the classical $N$-electron equilibrium configurations. Introducing the requirement of total wavefunction antisymmetry selects out the allowed minimum energy $N$-electron states. It is shown that low-energy minima can exist at filling factors $\nu = \frac{p}{2n+1}$ where $p$ and $n$ are any positive integers. These filling factors correspond to the experimentally observed Fractional (FQHE) and Integer (IQHE) Quantum Hall effects. The energy gaps calculated analytically at $\nu = \frac{p}{3}$ are found to be consistent with experimental data as a function of magnetic field, over a range of samples.
I. INTRODUCTION

The problem of a highly-correlated, two-dimensional electron gas in an external magnetic field has attracted much attention in the past decade. Of particular interest is the microscopic origin of the observed fractions in the Fractional Quantum Hall Effect (FQHE)\(^1\)–\(^3\). In the past few years, it has also been appreciated that many-body effects play a role in the formation of the gaps giving rise to the Integer Quantum Hall Effect (IQHE). As a complement to the experimental work in this subject, there have been many theoretical models proposed for both the FQHE and the IQHE. These range from field-theoretical treatments through to numerical, finite-size (\(N \leq 6\)) calculations. One of the most successful theoretical developments has been the proposal of trial wavefunctions by Laughlin and others\(^1\),\(^3\)–\(^5\) to describe the interplay of wavefunction antisymmetry and electron-electron repulsion that effectively allows electrons in the lowest Landau level to form a highly correlated electron liquid. A related development by Jain\(^6\) considers the construction of ‘composite’ fermions by attaching flux tubes to each electron – recent work on Chern-Simons field theories provides some support for such composite-fermion construction schemes\(^3\),\(^7\). The general problem of describing an \(N\)-electron gas in an external magnetic field has recently taken on additional importance in semiconductor physics due to the fabrication of quantum dots containing a finite number of electrons\(^8\)–\(^10\). It is interesting to note that although the FQHE was originally observed in infinite two-dimensional electron gases (2DEG), it even persists in quantum dots containing a large but finite number \(N\) of electrons\(^11\).

Given the fact that the underlying, microscopic \(N\)-electron Hamiltonian is known, one could ask whether there exists an alternative, more direct way of understanding the nature of highly-correlated electron states \emph{without} recourse to composite-fermion constructions, effective field theories, restrictions to lowest Landau levels and/or small numbers of electrons. The obvious stumbling blocks are that the electron-electron repulsion and the cyclotron energy are typically comparable in magnitude, and that \(N\)-electron Schrodinger equations are generally intractable analytically.

In this paper we pursue such an alternative approach starting with an \(N\)-electron
Schrodinger equation. We develop a microscopic, analytical theory describing correlated states of a confined $N$-electron gas in two dimensions subject to an external magnetic field $B$. The number of electrons $N$ and the strength of the electron-electron interaction can be arbitrarily large, and all Landau levels are included implicitly. We show that the description of $N$-electron correlated states at finite $B$ reduces to a universal effective problem which resembles a fictitious particle moving in a multidimensional space occupied by potential minima corresponding to the classical $N$-electron equilibrium configurations. Introducing the requirement of $N$-electron wavefunction antisymmetry selects out the allowed minimum energy $N$-electron states. A possible connection with the FQHE and IQHE is then proposed. In particular, it is argued that low-energy minima can form at particular angular momenta corresponding to filling factors $\nu = \frac{p}{2n+1}$ where $p$ and $n$ are any integer. These filling factors correspond to those observed experimentally in the FQHE and IQHE.

The present theory suggests the following possible physical interpretation of FQHE and IQHE states. Consider an $N$-electron wavefunction localized around a Wigner crystal (WX) configuration with total relative angular momentum $J$. At particular values of $J$, $N$-electron wavefunctions localized around nearby defect configurations (i.e. WX plus defect which we shall denote as WXD) can co-exist; we note that the allowed values of $J$ such that $N$-electron states can co-exist around WX and WXD simultaneously are severely restricted by the requirement of total wavefunction antisymmetry. At these common $J$ values, which we shall denote as $J = J_m$, hybridization of the $N$-electron states centered on the WX and WXD minima can occur. This hybridization effectively allows the electrons in the WX solid to diffuse throughout the system via WXD defect states. The resulting delocalized ‘liquid’-like $N$-electron state has a lower zero-point energy – a gap therefore opens up between the liquid-like states at $J = J_m$ and other states at $J \neq J_m$. For large $N$ the resulting liquid-like ground-states at $J = J_m$ have filling factors given by the well-known formula $\nu = \frac{N(N-1)}{2J_m}$. We find that the $\nu$ values at which these gaps arise are identical to those observed experimentally in the FQHE and IQHE. The energy gaps calculated analytically at
\[ \nu = \frac{k}{2} \] are found to be consistent with experimental data obtained from a range of samples. Various other known features of FQHE states can also be reproduced.

The model avoids discussion of one-electron properties such as Landau levels, and therefore offers the possibility of a unified description of both the FQHE and IQHE based on a microscopic \( N \)-electron Schrodinger equation. The formalism in this paper builds on an earlier model presented by us in Ref. 12. In particular, we conjectured in Ref. 12 that the classical minimum energy configurations play a crucial role in deciding the symmetry-allowed \( N \)-electron correlated states in few-electron quantum dots. It was pointed out that the classical minimum energy configurations for \( N < 6 \) all consist of \( N \) particles on a ring, while for \( N = 6 \) additional minima occur. Curiously, it is precisely at \( N = 6 \) that the magic number \( J \) sequence of \( \Delta J = N \) is broken. This idea was independently pursued by Maksym in a fascinating way for \( N \leq 6 \) – the classical Eckardt frame was employed to study correlated few-electron dynamics and, in particular, the possible existence of ‘liquid’-like states. We note that the term ‘liquid’-like was introduced by Maksym to describe the loss of symmetry occurring when states corresponding to different classical minima are allowed to mix. This terminology will also be used in the present paper. We wish to emphasize that the model presented here is qualitatively different from an earlier theoretical approach of Kivelson et al.\(^{16}\) based on the so-called cooperative ring exchange. In short, we are suggesting here that FQHE states are the liquid-like states resulting from the hybridization of \( N \)-electron wavefunctions localized around both crystal (WX) and crystal-plus-defect configurations (WXD).

The outline of the paper is as follows. In Sec. II we present the microscopic \( N \)-electron Schrodinger equation. The hyperangular coordinate system is introduced for the relative motion Hamiltonian. The problem then reduces to a \( 2N - 4 \) hyperangular equation (Sec. II.1). In Sec. II.2 the specific case of \( N = 3 \) is outlined. This was discussed in detail in Ref. 12 and is reviewed here since it is useful for visualizing the \( N \)-electron results. In Sec. II.3 a simplified hyperangular equation is obtained which is valid in the regime of strong electron-electron interactions and for large \( N \). The characteristics of the lowest energy solutions are
discussed. Section III addresses the requirement of $N$-electron wavefunction antisymmetry. Permutation symmetries of the $N$-electron wavefunction become space-group operations in the multi-dimensional hyperangular configuration space. The states which will become ground states separated by a finite energy gap are found to correspond to filling fractions observed in the FQHE. Section IV obtains analytic estimates for the FQHE gaps at the fractions $\frac{p}{3}$ as an example. These estimates are found to be consistent with experimental data over a range of samples, despite the fact that the results emerge from a simple one-dimensional, particle-in-a-box equation. Section V summarizes the results.

II. MICROSCOPIC $N$-ELECTRON HAMILTONIAN

The analytic tractability of our model is made possible by a combination of a parabolic confinement potential and an inverse-square electron-electron repulsion potential. The parabolic confinement is known to be a reasonable approximation for many semiconductor quantum dot samples. For the case of a heterostructure (i.e. 2DEG) it mimics the effect of a positive background yielding an approximately uniform electron density in the large $N$ limit (see Ref. 14). The $\beta/r^2$ electron-electron interaction ($\beta > 0$) is not unrealistic in quantum dots due to the presence of image charges in neighboring electrodes. Recent theoretical work suggests that the true repulsive interaction between electrons in a quantum dot dot is more likely to be proportional to $1/r^n$ with $n \sim 3$ at large $r$ and $n \sim 1$ at small $r$. In heterostructures, the electron-electron interaction is probably less affected by image-charge effects. However the general features of our results, which are based on the assumption that $n = 2$ for all $r$, should still be qualitatively useful. In particular, the occurrence of FQHE in two-dimensional electron gases is not thought to depend crucially on the precise form of the electron-electron repulsion. Recent quantitative comparisons have indeed shown that the $1/r^2$ and $1/r$ repulsive interactions yield $N$-electron energy spectra with very similar features. Of particular relevance to the present theory is the finding that the classical minimum energy configurations for $N$ electrons in a two-dimensional parabolic confinement potential seem to be almost identical for both $1/r$ and $1/r^2$ interactions.
The exact Schrödinger equation for \( N \) electrons with repulsive interaction \( \beta/r^2 \) moving in a 2D parabolic potential subject to a magnetic field \( B \) (symmetric gauge) along the z-axis, is given by \((H_{\text{space}} + H_{\text{spin}})\Psi = E\Psi\);

\[
H_{\text{space}} = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 |r_i|^2 \right) + \sum_{i<j} \frac{\beta}{|r_i - r_j|^2}
\]

\[
= \sum_{i=1}^{N} \left( \frac{p_i^2}{2m^*} + \frac{1}{2} m^* \omega_0^2(B) |r_i|^2 + \frac{\omega_c}{2} l_i \right) + \sum_{i<j} \frac{\beta}{|r_i - r_j|^2}
\]

\[ (1) \]

where \( \omega_0^2(B) = \omega_0^2 + \frac{\omega_c^2}{4} \), \( \omega_c \) is the cyclotron frequency, and \( H_{\text{spin}} = -g^* \mu_B B \sum_i s_{i,z} \). The momentum and position of the \( i \)'th particle are given by 2D vectors \( p_i \) and \( r_i \) respectively; \( l_i \) is the z-component of the angular momentum. The exact eigenstates are written in terms of products of spatial and spin eigenstates obtained from \( H_{\text{space}} \) and \( H_{\text{spin}} \) respectively.

Eigenstates of \( H_{\text{spin}} \) are just products of the spinors of the individual electrons and have energy \( E_{\text{spin}} = g^* \mu_B BS_z \), where \( S_z \) is the z-component of total spin and \( g^* \) is the electron effective \( g \)-factor. We employ standard Jacobi coordinates \( X_j \) \((j = 1, 2, \ldots, N)\) where \( X_1 = \frac{1}{N} \sum_j r_j \) (center-of-mass coordinate) and \( X_{j>1} \) (relative coordinates) is given by

\[
X_j = [j - \frac{1}{j}] \frac{1}{2} \left[ r_j - \frac{1}{j - 1} (r_1 + r_2 + \ldots r_{j-1}) \right]
\]

(2)

together with the conjugate momenta \( P_j \) (see Fig. 1 for \( N = 3 \)). The center-of-mass motion decouples, \( H_{\text{space}} = H_{\text{CM}}(X_1) + H_{\text{rel}}(\{X_{j>1}\}) \), hence \( E_{\text{space}} = E_{\text{CM}} + E_{\text{rel}} \). The exact eigenstates of \( H_{\text{CM}} \) and energies \( E_{\text{CM}} \) are well-known\[23\]. The non-trivial problem is to solve the relative motion equation \( H_{\text{rel}} \psi = E_{\text{rel}} \psi \). We transform the relative coordinates \( \{X_{j>1}\} \) to standard hyperspherical coordinates: \( X_j = r (\prod_{i=j+1}^{N} \cos \alpha_i) \sin \alpha_j e^{i\theta_j} \) with \( r \geq 0 \) and \( 0 \leq \alpha_j \leq \frac{\pi}{2} \) \((\alpha_2 = \frac{\pi}{2})\). Physically, the hyperradius \( r \) is just the root-mean-square electron-electron separation. The exact eigenstates of \( H_{\text{rel}} \) have the form \( \psi_{\text{rel}} = R(r)F(\Omega) \) where \( \Omega \) denotes the \((2N-3)\) hyperangular \( \{\theta; \alpha\} \) variables; \( R(r) \) and \( F(\Omega) \) are solutions of the hyperradial and hyperangular equations respectively. The hyperradial equation is given by

\[
\left[ \frac{d^2}{dr^2} + \frac{2N - 3}{r} \frac{d}{dr} - \frac{\gamma(\gamma + 2N - 4)}{r^2} - \frac{r^2}{l_0^4} + \frac{2m^*(E_{\text{rel}} - \hbar J \omega_c)}{\hbar^2} \right] R(r) = 0
\]

(3)
where $l_0^2 = \hbar(m^*\omega_0(B))^{-1}$ and $J$ is the total relative angular momentum. The parameter $\gamma > 0$ and is related to the eigenvalue of the $B$ and $\omega_0$-independent hyperangular equation (see Sec. II.1). Equation (3) can be solved exactly yielding

$$E_{\text{rel}} = \hbar\omega_0(B)[2n + \gamma + N - 1] + J\frac{\hbar\omega_c}{2}$$

(4)

where $n$ is any positive integer or zero and

$$R(r) = \left[\frac{r}{l_0}\right]^{\gamma}L_n^{\gamma+N-2}(\frac{r^2}{l_0^2})e^{-\frac{r^2}{2l_0^2}}.$$  

(5)

Equation (4) provides an exact and infinite set of relative breathing-mode excitations $2\hbar\omega_0(B)\Delta n$ for any $N$ regardless of particle statistics and/or spin states. These quantum breathing modes were first reported in Ref. 12, and later confirmed by Geller et al.\textsuperscript{24} – the classical version of these modes for the Coulomb interaction was discussed in detail by Schweigert et al.\textsuperscript{25}

II.1 Exact hyperangular equation for any $N$

It remains to solve the $B$ and $\omega_0$-independent hyperangular equation which is given by

$$[\Theta_N^2 + \frac{2m^*\beta}{\hbar^2}V(\Omega)]F(\Omega) = [\gamma(\gamma + 2N - 4)]F(\Omega)$$

(6)

where

$$\Theta_N^2 \equiv -\frac{\partial^2}{\partial\alpha_N^2} + \frac{2N - 6 - (2N - 4)\cos2\alpha_N}{\sin2\alpha_N} \frac{\partial}{\partial\alpha_N} + \sec^2\alpha_N\Theta_{N-1}^2 - \cosec^2\alpha_N\frac{\partial^2}{\partial\theta_N^2}.$$  

(7)

The quantity $V(\Omega)$ is given by $r^2\sum_{i<j}|\mathbf{r}_i - \mathbf{r}_j|^{-2}$ and only depends on hyperangular coordinates $\Omega \equiv \{\theta, \alpha\}$. We emphasize that this hyperangular equation (Eq. (6)) is universal in that it is independent of the values of the magnetic field or confinement: solving Eq. (6) for $\gamma$, and hence using Eq. (4), yields the complete solutions of the $N$-electron Hamiltonian $H$ for all magnetic fields and confinement strengths. Unfortunately the hyperangular equation does not admit exact solutions for $\gamma$. Sections II.2–4 will consider various approximations to Eq. (6) which make the problem tractable. Because $J$ remains a good quantum number, we can introduce a Jacobi transformation of the relative motion angles $\{\theta_i\}$: in particular
\[
\theta' = \frac{1}{N-1} \sum_{j=2}^{N} \theta_j
\] (8)

and

\[
\theta_{[j]} = \left[ \frac{j-2}{j-1} \right] \frac{1}{2} \left[ \theta_j - \frac{1}{j-2} (\theta_2 + \theta_3 + \ldots \theta_{j-1}) \right]
\] (9)

where \( j = 3, 4 \ldots N \). We hence have one \( \theta' \) variable, \((N - 2)\) \( \theta_{[j]} \) variables, \((N - 2)\) \( \alpha \) variables and one hyperradius \( r \) giving a total of \( 2N - 2 \) variables as required for the relative motion. The exact eigenstates of \( H_{\text{rel}} \) have the form \( \psi = e^{iJ \theta'} R(r) G(\Omega') \) where \( \Omega' \) denotes the \((2N - 4)\) \( \{\theta_{[j]}; \alpha_j\} \) variables excluding \( \theta' \). The term \( V(\Omega) \) is independent of \( \theta' \) and will hence be written as \( V(\Omega') \). It is useful to rewrite the eigenvalue of the hyperangular equation in terms of a new variable \( \epsilon \) as follows:

\[
\epsilon = \frac{\hbar^2}{8} \left[ \gamma (\gamma + 2N - 4) - J^2 - \frac{2m^*\beta}{\hbar^2} V(\Omega'_0) \right]
\] (10)

where \( V(\Omega'_0) \) is the value of \( V(\Omega') \) evaluated at the hyperangles corresponding to a particular classical, minimum-energy \( N \)-electron configuration (Wigner molecule). Permuting electron indices will provide a set \( \{\Omega'_i\} \) of symmetrically equivalent minima (SEM)\[22\] with the same potential energy \( V(\Omega'_i) \equiv V(\Omega'_0) \) for all \( i \) (e.g. \( \Omega'_0 \) and \( \Omega'_1 \) shown schematically in Fig. 2). Such SEMs have the same topological structure but cannot be transformed into each other by rotations\[22\]. As will be shown in Sec. II.2, there are two such SEMs for \( N = 3 \). The quantity \( \epsilon \) in Eq. (10) accounts for the contribution to the eigenvalue of the hyperangular equation without including either the contributions from the rigid-body rotational energy \( J^2 \) or the electrostatic potential energy \( \frac{2m^*\beta}{\hbar^2} V(\Omega'_0) \) of the classical minimum-energy configuration. Physically therefore, \( \epsilon \) contains the zero point energy in \( \Omega' \)-space associated with the quantum-mechanical spread of \( G(\Omega') \) about the minima \( \{\Omega'_i\} \). The actual spread in \( G(\Omega') \) and hence \( \epsilon \) will depend on the total wavefunction antisymmetry requirement. This is illustrated for \( N = 3 \) in Sec. II.2 and discussed for large \( N \) in Secs. II.3, II.4 and III. In general \( \epsilon \geq 0 \), \( \epsilon \sim \beta^\mu \) where \( \mu < 1 \), and \( \epsilon \sim J^\delta \) where \( \delta < 2 \): these statements will be illustrated in Sec. II.2 for \( N = 3 \). It is straightforward to show that the term \( \frac{2m^*\beta}{\hbar^2} V(\Omega'_0) \)
appearing in the definition of $\epsilon$ is identical to $[\frac{V_{\text{class}}(\omega_0)}{\omega_0}]^2$ where $V_{\text{class}}$ is the potential energy of the classical, minimum-energy $N$-electron configuration, thereby recovering the expression given in Ref. 12. Note that $V_{\text{class}} \propto \beta \frac{\epsilon^2}{\omega_0(B)}$ and that $\epsilon$ (like $\gamma$) is independent of $B$ and $\omega_0$. The exact relative energy for any $N$ can now be written as

$$E_{\text{rel}} = \hbar \omega_0(B)[2n + ([N-2]^2 + J^2 + \frac{2m^4\beta}{\hbar^2}V(\Omega_0') + \frac{8\epsilon}{\hbar^2})^2 + 1] + J\frac{\hbar \omega_c}{2} \tag{11}.$$

$E_{\text{rel}}$ only depends on particle statistics through $\epsilon$. As $\hbar \to 0$, $\epsilon \to 0$ and $E_{\text{rel}} \to V_{\text{class}}$.

The exact $E_{\text{rel}}$ expression has an important consequence. The $J$-dependence of $\epsilon$ is weaker than $J^2$ as $J \to 0$. Hence the term $J\frac{\hbar \omega_c}{2}$ in $E_{\text{rel}}$ will dominate the $J$-dependence of $E_{\text{rel}}$ for small $J$ at fixed magnetic field $\omega_c$. For states with $J < 0$, $E_{\text{rel}}$ will hence initially decrease as $|J|$ increases. On the other hand at large negative $J$, $E_{\text{rel}}$ will tend to $\hbar(\omega_0(B) - \frac{\omega_c}{2})|J|$ and hence will increase linearly with $|J|$ at a given $\omega_c$. This implies that $E_{\text{rel}}$ has a minimum at a finite negative $J$ for a given fixed magnetic field $\omega_c$. This is the basic mechanism behind the tendency of an $N$-electron gas to form ground states at increasingly large $J$ values as the magnetic field is increased. As will be shown in Sec. II.2 for $N = 3$ electrons, and in Sec. III for large $N$, only a subset of these $J$ minima are permitted under the requirement of total wavefunction antisymmetry. These $J$-values are often called ‘magic number’ $J$-values in the context of few-electron quantum dots. In Sec. III we will show that the analogous ‘magic number’ $J$ states for a large-$N$ electron gas constitute FQHE and IQHE states. We emphasize that so far our results are exact for any electron number $N$, electron-electron interaction strength $\beta$, magnetic field $\omega_c$ and parabolic confinement $\omega_0$.

II.2 Specific case of $N = 3$

This case was studied in Ref. 12. Here we will summarize the results since they are important for understanding the general $N$ case. For convenience we change variables from $\alpha, \theta$ (c.f. Fig. 1) to $x, y$ where $x = \ln[\tan(\frac{\pi}{2} - \alpha)]$ and $y = \theta - \frac{\pi}{2}$. Since $0 \leq \alpha \leq \frac{\pi}{2}$, hence $-\infty \leq x \leq \infty$ (N.B. $-\pi \leq y \leq \pi$). We define $p_x = \frac{h}{\tau} \frac{\partial}{\partial x}$ and $p_y = \frac{h}{\tau} \frac{\partial}{\partial y}$. The exact hyperrangular equation (Eq. (6)) now takes the form
\[
\left( \frac{p_x^2}{2} + \frac{p_y + \hbar \cos(2\tan^{-1}e^x)}{2} \right)^2 + V(x, y; \epsilon)G(x, y) = \epsilon G(x, y)
\]  
(12)

where

\[
V(x, y; \epsilon) = m^* \beta \left[ \frac{(2 + \cos(2\tan^{-1}e^x))}{\csc(2\tan^{-1}e^x) + \cot(\tan^{-1}e^x)^2} - 3\sin^2 y - \frac{3}{4} \sin^2(2\tan^{-1}e^x) \right. \\
\left. + \frac{1}{2} \cos^2(\tan^{-1}e^x) + \frac{\epsilon}{m^* \beta^2} \cos^2(2\tan^{-1}e^x) \right].
\]  
(13)

Equation (12) represents the single-body Hamiltonian for a fictitious particle of energy \( \epsilon \) and unit mass, moving in the xy-plane in a non-linear (i.e. \( \epsilon \)-dependent) potential \( V(x, y; \epsilon) \), subject to a fictitious, non-uniform magnetic field in the z-direction

\[
B_{\text{fic}} = \frac{\hbar J c}{4 e} [1 - \cos(4(\tan^{-1}e^x))].
\]  
(14)

\( B_{\text{fic}} \) is independent of \( B \) and has a maximum of \( \frac{\hbar J c}{2e} \) at \( x = 0 \) for all \( y \). For small \( x \), \( B_{\text{fic}} \approx \frac{\hbar J c}{2e}(1 - x^2) \). As \( x \to \pm \infty \), \( B_{\text{fic}} \to 0 \). Note we have here chosen to highlight the Schrödinger-like form of Eq. (12); a simple rearrangement of Eq. (12) shows it to be hermitian with a weighting function \( \sin^2(2\tan^{-1}e^x) \). These results are exact so far. Figure 3 shows the potential \( V(x, y; \epsilon) \) in the \((x, y)\) plane. \( V(x, y; \epsilon) \geq 0 \) everywhere. Minima occur at \((0, 0)\) and \((0, \pm \pi)\) where \( V(x, y; \epsilon) = 0 \) (N.B. \((0, \pi)\) is equivalent to \((0, -\pi)\)). Maxima occur at \((\ln \sqrt{3}, \pm \frac{\pi}{2})\) in Fig. 3, where \( V(x, y; \epsilon) \to \infty \). Since \( \epsilon \geq 0 \), these statements hold for any \( \epsilon \). We now discuss the physical significance of these features. The classical configurations of minimum energy (Wigner molecule) correspond to the particles lying on a ring in the form of an equilateral triangle with \( V_{\text{class}} = \omega_0(B)[6m^* \beta]^\frac{1}{2} \). There are two distinct configurations, i.e. two distinct symmetrically equivalent minima, with clockwise orderings \( \Omega_0 \equiv (132) \) and \( \Omega'_1 \equiv (123) \) corresponding to \((\alpha, \theta) = (\frac{\pi}{3}, \pm \frac{\pi}{6})\). In \((x, y)\) coordinates, these correspond to \((0, 0)\) and \((0, \pi)\) (equivalently, \((0, -\pi)\)). Hence the classical configurations coincide with the minima in \( V(x, y; \epsilon) \) in Fig. 3 and the maximum in \( B_{\text{fic}} \). As pointed out in Ref. 12, the formation of a Wigner molecule should therefore be favored by both large \( B_{\text{fic}} \) (i.e. large \( |J| \)) and deep \( V(x, y; \epsilon) \) minima (i.e. large \( \beta \), strong electron-electron interactions).

Consider the limit of very strong electron-electron interactions (i.e. \( \beta \to \infty \)). Since the tunnel barrier height between the two \( V(x, y; \epsilon) \) minima \( \sim \beta \), the fictitious particle sits at
one of these minima and the system is locked in one of the two classical configurations, e.g. \( \Omega'_0 \equiv (132) \) at \((0,0)\). The tunnelling probability between the minima \( \Omega'_0 \) and \( \Omega'_1 \) is zero. Tunnelling between the two minima implies a mixture of configuration \((123)\) into \((132)\) and hence interchange of the original electrons; in many-body language exchange effects arising from wavefunction antisymmetry are therefore negligible. \( \epsilon \) is small compared to \( m^*\beta \) and Eq. (12) reduces to

\[
E_{\text{rel}} = \hbar \omega_0(B)[2n + (1 + J^2 + \frac{6m^*\beta}{\hbar^2})\frac{h}{2} + 1] + J\frac{\hbar \omega_c}{2}.
\] (15)

The energy \( E_{\text{rel}} \geq V_{\text{class}} \) since it includes the hyperradial zero-point energy (N.B. \( \hbar \rightarrow 0 \) yields \( E_{\text{rel}} \rightarrow V_{\text{class}} \) and \( B_{\text{fic}} \rightarrow 0 \)).

Next consider large but finite \( \beta \). The fictitious particle now moves in the vicinity of the minimum \( \Omega'_0 \) (i.e. \((x,y) \approx (0,0)\)). The electrons in the Wigner solid are effectively vibrating around their classical positions. Expanding the potential \( V(x,y;\epsilon) \) about \((0,0)\) to third order, the exact Eq. (12) becomes

\[
[\frac{p_x^2}{2} + (\frac{p_y - \frac{\hbar J}{2}}{2})^2 + \frac{1}{2}\omega_x^2 x^2 + \frac{1}{2}\omega_y^2 y^2]G(x,y) = \epsilon G(x,y)
\] (16)

where \( \omega_x^2 = \left(\frac{3m^*\beta}{4} + 2\epsilon\right) \) and \( \omega_y^2 = \frac{3m^*\beta}{4} \). This has the form of a single electron moving in an anisotropic parabolic potential, subject to a uniform magnetic field \( B_{\text{fic}} = \frac{\hbar J}{2e} \). Equation (16) is exactly solvable for \( \epsilon \) using a symmetric gauge \(^{19}\) (the energies are independent of the choice of gauge for \( B_{\text{fic}} \)). As an illustration, we consider small \( \epsilon \) hence \( \omega_x \approx \omega_y \). The relative energy is then given by

\[
E_{\text{rel}} = \hbar \omega_0(B)(2n + [1 + J^2 + \frac{6m^*\beta}{\hbar^2} + 2(2n' + |l'| + 1)(J^2 + \frac{12m^*\beta}{\hbar^2})\frac{h}{2} + 2l'J]\frac{h}{2} + 1) + J\frac{\hbar \omega_c}{2}.
\] (17)

The fictitious particle has its own set of Fock-Darwin (and hence Landau) levels \(^{23}\) labelled by \( n' \) and a ficticious angular momentum \( l' \). For large \( \beta \) and small \( n',l' \) and \( J \), Eq. (17) yields an oscillator excitation spectrum with two characteristic frequencies \( \sqrt{2\hbar \omega_0(B)} \) and \( 2\hbar \omega_0(B) \) representing shear and breathing modes of the Wigner molecule.
For smaller $\beta$ (i.e. weaker interactions) and/or larger $\epsilon$ (i.e. excited states), the tunneling probability between the $V(x, y; \epsilon)$ minima $\Omega'_0$ and $\Omega'_1$ in Fig. 3 becomes significant. The Wigner molecule begins to melt and wavefunction antisymmetry must be included. This is discussed further in Sec. III. As mentioned in Ref. 12, the resulting analytically obtained magic-number $J$ transitions are found to be in good agreement with the numerical results for $1/r$ interaction. We note that the analytic results become more accurate in the Wigner solid regime (e.g. large $\beta$ or $|J|$) while the numerical calculations become more computationally demanding.

II.3 Simplified hyperangular equations for arbitrarily large $N$

For general $N$ the hyperrangular equation (Eq. (6)) is $(2N - 4)$-dimensional. However in the Wigner solid regime (large $\beta$ or $|J|$) the classical minimum energy configurations will still be important in determining $\epsilon$ and hence $E_{\text{rel}}$, just as for $N = 3$. Here we will consider the limit that the number of electrons is large ($N >> 1$). This is the limit of interest in the FQHE and in large quantum dots. Specifically, we will introduce in this section a series of approximations in order to simplify the exact hyperangular equation. At each stage, the corresponding simplified hyperangular equation is explicitly given. The resulting discussion is detailed – however we feel that this is necessary in order to justify the successively simpler (and more approximate) hyperangular equations. Each of these simplified hyperangular equations can be solved numerically: the complexity of the algorithms needed obviously decreases as more approximations are introduced. However, the goal in this paper is to obtain a simplified version of the hyperangular equation which can be treated analytically, but which is still based on a set of reasonable approximations.

Figure 4 shows the classical ground-state configuration for $N = 230$ electrons (black dots) in a parabolic quantum dot, as obtained by Bedanov and Peeters using a Monte Carlo algorithm. The rings are drawn as a guide to the eye. The number $N$ of electrons is relatively small in the context of the $N \to \infty$ limit and hence the details of the ground-state configuration, particularly for larger rings, will be prone to edge effects. However, the inner
rings show a nearly hexagonal lattice as expected for the $N \to \infty$ limit. For the purposes of illustration we will therefore consider Fig. 4 as being representative of the $N \to \infty$ classical configuration. Consider the particular classical configuration $\Omega'_0$ where the $N$’th electron is near the center and the first electron is on the circumference of the droplet. This is shown schematically in Fig. 5. As discussed in Sec. II.2 for $N = 3$, the fully quantum mechanical system will also lie near this configuration in $\Omega'_0$-space in the limit of very large $\beta$. The $j$’th Jacobi coordinate is given by

$$X_j = \left[ \frac{j-1}{j} \right]^2 (r_j - R_{j-1}) \quad (18)$$

where $R_{j-1} = \frac{1}{j-1}(r_1 + r_2 + \ldots r_{j-1})$: this quantity $R_{j-1}$ can be thought of as the ‘center-of-mass’ of the electrons $1, 2, \ldots j - 1$. For $j >> 1$, and for configurations as in Figs. 4 and 5 where the electrons are evenly distributed around the origin, the quantity $R_{j-1}$ will be small compared to the typical electron lattice spacing. In addition, the prefactor $\left[ \frac{j-1}{j} \right]^2 \to 1$ for large $j$. Hence $X_j \to r_j$ for large $j$. However, there is an exact identity for hyperangular Jacobi coordinates: $\sum_{j=2}^{N} |X_j|^2 = 1$. Given that $X_j \to 0$ as $j \to N$ for large $N$, this implies that each term $\left| \frac{X_j}{r_j} \right|^2 << 1$ for large $j$. Given the definition of the hyperangular coordinates stated earlier on, it follows that the hyperangles $\alpha_j << 1$ for $j >> 1$. Hence to first order in $\alpha_j$, we can approximate $X_N = r \sin \alpha_N \approx r \alpha_N$. Similarly $X_{N-1} = r \cos \alpha_N \sin \alpha_{N-1} \approx r \alpha_{N-1}$ and, more generally, $X_j \approx r \alpha_j$. To summarize, for configurations similar to that shown in Fig. 5, we have the approximate result $X_j \approx r \alpha_j e^{i \theta_j}$ in the $N >> 1$ and $j >> 1$ limit.

There are two points to note: although we need both $j >> 1$ and $N >> 1$, $j$ can still be an order of magnitude less than $N$. Second, the error introduced by assuming $\sin \alpha_j \approx \alpha_j$ is still reasonably small even for $j = 2$ (recall $\alpha_2 = \frac{\pi}{2} \approx 1.57$ as compared to $\sin \alpha_2 = 1$.

To remain consistent within our approximation, we will take $\alpha_2 = 1$ instead of $\frac{\pi}{2}$ in what follows).

This approximate form for $X_j$ leads to an interesting simplification of the exact hyperangular equation. The small-angle (i.e. $\alpha_j << 1$) limit of Eq. (6) yields:
\[ [\sum_{j=2}^{N} -\frac{\hbar^2}{2m^*} \nabla_j^2 + \beta V(\Omega)]F(\Omega) = \frac{\hbar^2}{2m^*} \gamma (\gamma + 2N - 4) F(\Omega) \]  \hspace{1cm} (19)

where

\[ \nabla_j^2 \equiv -\frac{\partial^2}{\partial \alpha_j^2} - \frac{1}{\alpha_j} \frac{\partial}{\partial \alpha_j} - \frac{1}{\alpha_j^2} \frac{\partial^2}{\partial \theta_j^2} \]  \hspace{1cm} (20)

is the two-dimensional Laplacian for a fictitious particle with position \((\alpha_j, \theta_j)\) in polar coordinates, the potential energy term

\[ V(\Omega) \equiv V(\Omega') \sim \sum_{j<j'} |\alpha_j e^{i\theta_j} - \alpha_{j'} e^{i\theta_{j'}}|^2 \]  \hspace{1cm} (21)

and \(F(\Omega) = e^{iJ\theta'}G(\Omega')\). This equation is a good approximation for \(j \to N\) with \(N \gg 1\) but becomes worse as \(j \to 0\) and/or \(N \to 0\). (Recall \(\alpha_2 = 1\) hence the sum can start from \(j = 2\) as shown). However this is sufficient for the purposes of this paper since we are interested in states that evolve within the bulk of the \(N\)-electron droplet as opposed to those at the edge. Physically, Eq. (19) describes a set of \(N - 1\) fictitious particles moving on a two-dimensional plane subject to a two-body inverse-square interaction, in the absence of a magnetic field. It is interesting to note this transformation of having replaced an \(N\)-particle problem in a magnetic field with an \(N - 1\) particle problem without a magnetic field seems reminiscent of composite fermion constructions at half-integer filling fractions. The effective Schrodinger equation in Eq. (19) carries the following constraint: the exact hyperangular identity \(\sum_{j=2}^{N} \frac{X_j^2}{r^2} = 1\) implies \(\sum \alpha_j^2 \sim 1\). This may complicate any attempt at a solution using a ‘renormalization’ type of approach, such as the setting up of a recursion equation relating \(\gamma\) for \(N\) particles to \(\gamma\) for \(N - 1\).

It is more useful to view Eq. (19) in the context of a single ficticious particle moving in a multi-dimensional space containing potential miminima corresponding to the various classical minimum energy configurations \(\{\Omega_i\}\). This directly connects the \(N\)-electron problem to the \(N = 3\) problem discussed in Sec II.2. As discussed in Sec. II.1, a Jacobi transformation can be undertaken on the \(\{\theta_j\}\) variables. In particular,

\[ \theta_{[j]} = [j \frac{j-2}{j-1}]^2 (\theta_j - \Theta_{j-1}) \]  \hspace{1cm} (22)
where \( j = 3, 4 \ldots N \) and \( \Theta_{j-1} = \frac{1}{j-2} (\theta_2 + \theta_3 + \ldots \theta_{j-1}) \). The quantity \( \Theta_{j-1} \) represents the average of the angles \( \theta_j \) where \( j = 2, 3 \ldots j-1 \). For \( j >> 1 \) the quantity \( \Theta_{j-1} \) will be approximately a constant, \( \bar{\Theta} \), since the \( j-1 \) particles are evenly distributed about the origin in a given \( \Omega'_i \) configuration (recall Figs. 4 and 5). In addition, the prefactor \( [\frac{j-2}{j-1}]^{\frac{1}{2}} \rightarrow 1 \) for large \( j \). Hence \( \theta_{[j]} \rightarrow \theta_j - \bar{\Theta} \) for large \( j \), neglecting terms of order \( (\frac{1}{N}) \). With \( F(\Omega) = e^{iJ\bar{\theta}'}G(\Omega') \), Eq. (19) further reduces to

\[
\left[ \sum_{j=3}^{N} \frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \alpha_j^2} + \frac{1}{\alpha_j} \frac{\partial}{\partial \alpha_j} + \frac{1}{\alpha_j^2} \left[ \frac{\partial}{\partial \theta_{[j]}} + \frac{iJ}{N-1} \right]^2 \right) \right] \beta V(\Omega') G(\Omega') = \frac{\hbar^2}{2m^*} \gamma (\gamma + 2N - 4) G(\Omega')
\]

(23)

Again this equation is a good approximation for \( j \rightarrow N \) but becomes worse as \( j \rightarrow 0 \). The \( \{\theta_{[j]}; \alpha_j\} \) manifold carries the following constraints: \( \sum \alpha_j^2 \sim 1 \) and \( \sum \frac{\partial}{\partial \theta_{[j]}} \sim 0 \). The latter condition is an approximate identity for large \( N \) and is obtained by combining \( \sum \frac{\partial}{\partial \theta_{[j]}} = \frac{\partial}{\partial \theta'} \) (this is an exact property of any Jacobi transformation) and \( \frac{\partial}{\partial \theta_{[j]}} \sim \frac{\partial}{\partial \theta_{[j]}} + \frac{1}{N-1} \frac{\partial}{\partial \theta'} \). This new condition hence reflects the fact that the total relative angular momentum is only associated with the \( \theta' \) variable: there is no additional contribution to the relative angular momentum contained within the \( \Omega' \) dynamics. These approximate constraints allow us to make a further simplification of the hyperangular equation as follows. Using the approximate identity \( \sum \alpha_j^2 \sim 1 \) we can define an average hyperangle \( \bar{\alpha} \sim N^{-\frac{1}{2}} \). We will therefore replace the term \( \sum \frac{1}{\alpha_j^2} \frac{J^2}{(N-1)^2} \) in Eq. (23) by \( \frac{1}{\bar{\alpha}^2} \sum (\frac{J^2}{(N-1)^2} \sim J^2 \) assuming large \( N \). We can hence rewrite Eq. (23) in the form

\[
\left[ \sum_{j=3}^{N} \frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \alpha_j^2} + \frac{1}{\alpha_j} \frac{\partial}{\partial \alpha_j} + \frac{1}{\alpha_j^2} \left[ \frac{\partial^2}{\partial \theta_{[j]}^2} + \frac{2iJ}{N-1} \frac{\partial}{\partial \theta_{[j]}} \right] \right) \right] \beta [V(\Omega') - V(\Omega'_0)] G(\Omega') =
\]

\[
\frac{\hbar^2}{2m^*} [\gamma (\gamma + 2N - 4) - J^2 - \frac{2m^* \beta}{\hbar^2} V(\Omega'_0)] G(\Omega')
\]

(24)

Although its derivation has involved approximations, Eq. (24) merits some discussion since it elucidates several of the statements made in Sec. II.1. The right-hand side is just \( \frac{4}{m^*} \epsilon \). Given that \( \sum \alpha_j^2 \sim 1 \) and \( \sum \frac{\partial}{\partial \theta_{[j]}} \sim 0 \), the \( J \)-dependence of \( \epsilon \) will tend to be weaker than \( J^2 \)
as claimed earlier. Note that since \( \sum \alpha_j^2 \sim 1 \), the moment of inertia \( I \) of a given classical configuration in \( \Omega \)-space, treated as a rigid body, is just \( m^* \). Hence the classical rigid-body rotational energy \( \frac{\hbar^2 j^2}{2I} \sim \frac{\hbar^2 J^2}{2m^*} \) which is precisely the term appearing in the right-hand side of Eq. (24). This then justifies the statement made in Sec. II.1 that \( \epsilon \) excludes the classical rigid-body rotational energy. The term \( V(\Omega'_0) \) denotes \( V(\Omega') \) evaluated at a given classical SEM equilibrium configuration \( \Omega' \equiv \Omega'_0 \). We emphasize that \( V(\Omega'_0) \equiv V(\Omega'_0) \), i.e. same potential energy for all SEMs. Since \( \Omega'_0 \) is a minimum, the difference term \( [V(\Omega') - V(\Omega'_0)] \) can be expanded around \( \Omega'_0 \). The leading terms will be quadratic in \( \theta_{[j]} - \theta_{[j0]} \) etc. Hence \( \epsilon \) does indeed describe the zero-point energy associated with the spread in \( G(\Omega') \) around the classical minima, as claimed in Sec. II.1 and shown explicitly for \( N = 3 \) in Sec. II.2. This point is further discussed below for large \( N \).

The hyperangular equation Eq. (24) is now simpler, however it is still not quite in a form which makes it amenable to analytic calculation. This final step can be achieved with the following considerations. Given the two approximate constraints \( \sum \alpha_j^2 \sim 1 \) and \( \sum \frac{\partial}{\partial\theta_{[j]}} \sim 0 \), the term involving \( \sum \frac{1}{\alpha_j^2} \frac{\partial^2}{\partial\theta_{[j]}^2} \) should be small as compared to the term involving \( \frac{1}{\alpha_j^2} \frac{\partial^2}{\partial\theta_{[j]}^2} \), and hence will be neglected. Furthermore just as for \( N = 3 \), we are initially considering the quantum mechanical solution near a given classical minimum \( \Omega'_0 \), i.e. \( \beta \rightarrow \infty \). Hence the term \( \frac{1}{\alpha_j^2} \frac{\partial^2}{\partial\theta_{[j]}^2} \) can be approximated by \( \frac{1}{\alpha_{j0}} \frac{\partial^2}{\partial\theta_{[j]}^2} \) where \( \alpha_{j0} \) is the value of \( \alpha_j \) at \( \Omega' \equiv \Omega'_0 \). The fact that \( \Omega'_0 \) is a minimum suggests that the leading order expansion of \( [V(\Omega') - V(\Omega'_0)] \) will involve terms like \( (\theta_{[j]} - \theta_{[j0]})^2 \) and \( (\alpha_j - \alpha_{j0})^2 \) for all \( j \) but not cross terms: this was demonstrated explicitly for \( N = 3 \) earlier where \( V(x, y) \) was found to be a function of \( x^2 \) and \( y^2 \) but not \( xy \). This implies the following simplification for \( \Omega' \sim \Omega'_0 \): \( [V(\Omega') - V(\Omega'_0)] \sim \sum_j [v(\alpha_j - \alpha_{j0}) + w(\theta_{[j]} - \theta_{[j0]})] \) where both \( v \) and \( w \) have a minimum at \( \Omega' \equiv \Omega'_0 \), i.e. at \( \alpha_j = \alpha_{j0} \) and \( \theta_{[j]} = \theta_{[j0]} \). The approximate separability of the potential suggests that the hyperangular function \( G(\Omega') \) can now be written as \( f(\{\alpha_j - \alpha_{j0}\})g(\{\theta_{[j]} - \theta_{[j0]}\}) \) where the functions \( f \) and \( g \) are peaked around \( \Omega' \equiv \Omega'_0 \). This was shown to be true explicitly for \( N = 3 \) where \( f \) and \( g \) turned out to be gaussians (harmonic oscillator wavefunctions). Since \( \Omega'_0 \) is still a minimum point for large \( N \), \( f \) and \( g \) will retain their gaussian-like character for
general \( N \). We will therefore write \( g(\{\theta_{[j]} - \theta_{[j_0]}\}) \sim \prod_j g_j(\theta_{[j]} - \theta_{[j_0]}) \) where \( g_j(\theta_{[j]} - \theta_{[j_0]}) \) is a function peaked around the minimum coordinate \( \theta_{[j]} = \theta_{[j_0]} \). The hyperangular equation is now fully separable into an equation involving \( \{\alpha_j\} \)

\[
\left[ \sum_{j=3}^{N} - \frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \alpha_j^2} + \frac{1}{\alpha_j \partial \alpha_j} \right) + \beta v_j(\alpha_j - \alpha_{j_0}) \right] f(\{\alpha_j - \alpha_{j_0}\}) = E_\alpha f(\{\alpha_j - \alpha_{j_0}\})
\]

(25)

together with the following equations for each \( \theta_{[j]} \):

\[
\left[ - \frac{\hbar^2}{2m^* \alpha_{j_0}^2 \partial \theta_{[j]}^2} + \beta w_j(\theta_{[j]} - \theta_{[j_0]}) \right] g_j(\theta_{[j]} - \theta_{[j_0]}) = e_j g_j(\theta_{[j]} - \theta_{[j_0]})
\]

(26)

The relation between \( \epsilon \), \( E_\alpha \) and \( e_j \) is as follows: \( \frac{4}{m^*} \epsilon = E_\theta + E_\alpha \) where \( E_\theta = \sum_j e_j \). The full expression for the relative energy hence becomes

\[
E_{\text{rel}} = \hbar \omega_0(B)[2n + ([N - 2]^2 + J^2 + \frac{2m^* \beta}{\hbar^2} V(\Omega_0') + \frac{2m^*}{\hbar^2} [E_\theta + E_\alpha])^{\frac{1}{2}} + 1] + J \frac{\hbar \omega_c}{2}.
\]

(27)

Since Eqs. (25) and (26) have a Schrodinger-like form with \( E_\alpha \) and \( e_j \) as eigenvalues respectively, we will refer to these two quantities as ‘energies’ even though this is not strictly correct terminology.

**II.4 Characteristics of the low-energy solutions \( G(\Omega') \)**

So far we have considered the solutions near a particular minimum configuration \( \Omega_0' \), i.e. we have considered very large \( \beta \) just as we did initially for \( N = 3 \). Very large \( \beta \) implies that \( G(\Omega') \) will be peaked around one of the SEMs, e.g. around \( \Omega_0' \). In the limit of zero tunnelling between SEMs, the solution \( G(\Omega') \sim f(\{\alpha_j - \alpha_{j_0}\}) g(\{\theta_{[j]} - \theta_{[j_0]}\}) \) centered around \( \Omega_0' \) will be *degenerate* with the identically localized solutions centered at all other SEMs \( \{\Omega_i'\} \).

These localized functions can be thought of as atomic-like orbitals in \( \Omega' \) space. In particular there will be a set of orbitals associated with each SEM \( \Omega_i' \). The corresponding coordinates and hyperangular equations describing these solutions are identical to those obtained earlier in Sec. II.3: however the spatial ordering of the electrons for the various \( \Omega_i' \) minima will necessarily change; for example electron \( N \) will not necessarily be close to the center. Using the usual variational argument for Schrodinger-like equations, the lowest energy (i.e. lowest
\( E_\alpha \) and \( E_\theta \) solutions of Eqs. (26) and (27) will be those with the minimum number of nodes.

For large but finite \( \beta \) there will be a small but finite tunnelling between the various minima \( \{\Omega_i'\} \), hence the complete solution \( G(\Omega') \) will be more correctly described as a linear combination of the atomic-like solutions, just as in a single-particle tight-binding model. Furthermore for \( N \geq 6 \), as noted earlier, there will be additional classical minima which are not topologically equivalent; again borrowing from the language of molecular physics\(^{15,22}\) these minima are termed \textit{symmetrically inequivalent minima} (SIM). These SIMs are local minima in \( \Omega' \)-space which are often just slightly higher in energy than the SEMs \( \{\Omega_i\} \). In the large \( N \) limit, these minima correspond to defect states in a hexagonal crystal. Fisher, Halperin and Morf\(^{26}\) showed that a Wigner crystal with a localized defect (WXD) can be quite close in energy to the perfect Wigner crystal (WX). This finding was recently verified in the context of \( N \) electrons in a two-dimensional parabolic quantum dot by Bolton\(^3\) and Bedanov et al.\(^{14}\). These authors all found that the global minimum for the classical \( N \)-electron system tends towards a hexagonal crystal as \( N \to \infty \), as expected for the Wigner crystal (WX). However configurations corresponding to a Wigner crystal with single defects (WXD) are only slightly higher in energy. In the language of the present paper the WX represents the SEMs while the WXD represents the SIMs. Although the SIMs are not true global minima, the complete solution \( G(\Omega') \) should certainly include finite mixing with them. This is particularly true since the ‘nearest-neighbors’ of a given SEM in \( \Omega' \)-space are SIMs. This is simply a consequence of the fact that translation between two adjacent SEMs in \( \Omega' \)-space requires interchange of at least two electrons, while translation between a given SEM and its nearest SIMs requires only slight electron distortion. Each SEM minimum \( \Omega_i \) will have \( p \) defect states as its nearest neighbors in \( \Omega' \)-space – we denote these nearby SIM minima as \( \{\Omega'_i; a\} \) where \( a = 1, 2 \ldots p \) (c.f. Fig. 2).

The resulting wavefunction \( G(\Omega') \) will therefore resemble a tight-binding LCMO (Linear Combination of Molecular Orbitals) wavefunction where each ‘molecule’ consists of ‘atomic’ orbitals on one of the SEM minima \( \Omega_i \) mixed with ‘atomic’ orbitals on each of its nearby
SIM minima. We emphasize that \( N = 3 \) has no SIM minima. \( N = 6 \) is the smallest \( N \) having SIMs. The SIMs for \( N = 6 \) consist of a six-member ring configuration while the SEM’s contain a five-member ring plus one electron at the center. For general \( N \), the low-energy solutions should therefore be reasonably well-described by

\[
G(\Omega') \sim \sum_i \sum_a c_{i,a} f(\{\alpha_j - \alpha_{j;i,a}\}) g(\{\theta_{[j]} - \theta_{[j;i,a]}\}) .
\]

(28)

It is well-known from elementary tight-binding theory that the lowest-energy states are ‘bonding’ wavefunctions of \( s \)-orbitals. In the present context, we similarly expect the lowest energy \( G(\Omega') \) to have as few nodes as possible (i.e. it will be gaussian-like around each of the SEM \( \{\Omega'_i\} \) thereby resembling an \( s \)-orbital); it will also correspond to the coefficients \( c_{i,a} \) being identical for each \( i \) (i.e. it will resemble a ‘bonding’ state).

### III. FERMION STATISTICS, MAGIC NUMBERS AND FILLING FRACTIONS

So far we have not introduced the requirement that the total \( N \)-electron wavefunction be antisymmetric. In this section, we will show that it is precisely this requirement that produces the observed FQHE filling factors for large \( N \).

It is useful to first discuss the effect of antisymmetry in the case of \( N = 3 \) electrons before considering large \( N \). For three spin-polarized electrons, \( \psi \) must be antisymmetric under particle interchange \( i \leftrightarrow j \). The hyperradial part \( R(r) \) is invariant; particle permutation operations in \( (r_1, r_2, r_3) \) become straightforward space-group operations in the \( (x,y) \) plane. For small \( (x,y) \), \( 1 \leftrightarrow 2 \) is equivalent to \( (x, y) \rightarrow (x, y + \pi) \) with \( \theta' \rightarrow \theta' + \frac{\pi}{2} \); \( 1 \leftrightarrow 3 \) is equivalent to \( (x, y) \rightarrow (\bar{x}, \bar{y} - \pi) \) with \( \theta' \rightarrow \theta' + \frac{\pi}{6} \) (\( (\bar{x}, \bar{y}) \) represents \( (x, y) \) rotated by \( \frac{4\pi}{3} \)); \( 2 \leftrightarrow 3 \) is equivalent to \( (x, y) \rightarrow (\bar{x}, \bar{y} + \pi) \) with \( \theta' \rightarrow \theta' - \frac{\pi}{6} \) (\( (\bar{x}, \bar{y}) \) represents \( (x, y) \) rotated by \( -\frac{4\pi}{3} \)). The solutions \( G(x, y) \) of Eq. (12) with the lowest possible \( \epsilon \) and hence lowest \( E_{rel} \) at a given \( \omega_c \), should be nodeless in the vicinity of \( (0, 0) \) (c.f. ground state in the parabolic potential with \( n' = 0 = l' \) in Eq. (17)). However the above symmetry requirements forbid such a nodeless solution unless \( e^{i\frac{2\pi}{3}} = 1 \). Therefore the only symmetry-allowed solutions
$G(x, y)$ which are nodeless are those where $J$ is a multiple of three, as observed in numerical calculations for $N = 3$ electrons with a $1/r$ interaction. It is important to note that this condition, i.e. $e^{i\pi \frac{2J}{3}} = 1$, just arises from combining the effect of any two sets of particle interchanges $i \leftrightarrow j$. For $N = 3$, two sets of particle interchanges correspond to rotations of a given SEM: this can be seen simply as follows. Consider a given SEM in Fig. 3, e.g. $\Omega'_0 \equiv (132)$. Interchanging $1 \leftrightarrow 2$ and $2 \leftrightarrow 3$ yields the same SEM, i.e. $(132)$, rotated anticlockwise by $\frac{2\pi}{3}$. Hence combinations of two sets of particle interchanges merely rotate the Wigner molecule without involving a transformation from one SEM to another, i.e. without moving from $(132)$ to $(123)$. Hence in order to obtain the ‘magic’ angular momentum values for $N = 3$, it is sufficient to consider the subset of particle interchanges from the $S_3$ permutation group which correspond to point-group rotations $C_3$, i.e. those which do not correspond to translations between SEMs. This result is discussed by Maksym in Ref. 15 following earlier work on molecules by Wilson. Maksym also argued for $N = 3$ that the remaining permutations which correspond to translations between SEMs, and hence the effect of tunnelling between SEMs, represents a small perturbation which does not affect the magic $J$-values. In contrast, for $N = 6$ where topologically distinct classical configurations coexist, the tunnelling between SEMs and SIMs plays a crucial role in determining the $J$ values of the low-energy ground states of the system. In particular, Maksym pointed out that tunnelling between SEMs and SIMs should be most favorable when the SEM and SIM configurations have a common $J$ value. This is consistent with analogous ideas in single-particle tight-binding theory, where the overlap matrix element (and hence bandwidth) is larger between $s$ orbitals than between $s$ and $p$ orbitals. Maksym conjectured that the resulting tunnelling might lead to ‘liquid’-like states with a lower overall energy.

These considerations motivate us to follow a similar strategy for $N$ electrons. In particular, we will show that considering just a subset of particle interchanges of $S_N$ corresponding to rotations of rings within the Wigner molecule (WX) and Wigner molecule plus defect (WXD) is sufficient to determine the magic $J$-values corresponding to the observed FQHE filling factors. As for $N = 3$, we focus on the vicinity of a given SEM, e.g. $\Omega'_0$. Following
the discussion in Sec. II.3, interchanging \( r_i \leftrightarrow r_j \) is relatively straightforward for \( i, j \gg 1 \) since \( X_j \approx r \alpha_j e^{i \theta_j} \approx r_j \). Neglecting terms of order \( \frac{1}{N} \), it just corresponds to \( \alpha_i \leftrightarrow \alpha_j \) and \( \theta_i \leftrightarrow \theta_j \). The derivation of the transformation rules including terms of order \( \frac{1}{N} \), is straightforward but tedious. Just as for \( N = 3 \), however, it turns out in what follows that we do not need to consider individual \( i \leftrightarrow j \) transformations.

III.1 Spin-polarized system

Consider the classical configuration \( \Omega'_0 \) shown in Figs. 4 and 5. For large \( j \) the electrons can be thought of as forming an approximately ring-like structure. Counting the number of rings from the center outwards, the first ring contains 6 electrons, the second contains approximately 12 and so on. We first focus on a ‘typical’ ring without any defects: it will contain a large, even number \( N_m \) of electrons (approximately \( 6m \) electrons where \( 6m \gg 1 \)) but these electrons will have an index \( j \gg 1 \), i.e. we are not considering rings near the edge of the \( N \)-electron droplet. We are going to consider just the subset of all particle interchanges \( i \leftrightarrow j \) which are equivalent to rotations of this \( m \)'th ring. Since \( X_j \approx r \alpha_j e^{i \theta_j} \approx r_j \), all members of the ring have approximately the same \( \alpha \), i.e. \( \{ \alpha_j \} \equiv \alpha_m \) for all \( j \) in ring \( m \). Hence interchanging two members of the ring just involves a transformation between their \( \theta_j \) coordinates. Since all members of the ring have a similar environment and the same \( \alpha_j \), the potential energy \( w_j \) and hence \( g_j \) in Eq. (26) will have the same form for all \( j \) in the ring \( m \). As for \( N = 3 \), the lowest-energy solutions should be those with \( g_j \) nodeless; \( g_j \) will be an approximately gaussian function of \( \theta_{[j]} \) centered around \( \theta_{[j_0]} \). Hence we can write \( g_j \equiv g_m \) for all \( j \) in ring \( m \). We now rotate the electrons in the ring, and hence the ring itself, by an angle \( \frac{2 \pi}{N_m} \). Since \( X_j \sim r_j \) this corresponds to \( \theta_j \rightarrow \theta_j + \frac{2 \pi}{N_m} \). The \( g_m \) functions are nodeless and (in a given ring) identical, hence the product \( \prod_j g_j(\theta_{[j]} - \theta_{[j_0]}) \) for \( j \) in ring \( m \) can be replaced by \( \prod_j g_m(\theta_{[j]} - \theta_{[j_0]}) \). The transformation keeps the system within the subset of all SEMs corresponding to the same ring ordering, i.e. just as for \( N = 3 \) the rotation operation in real space becomes a space-group operation in \( \Omega' \)-space which translates the system between SEMs. Recall that \( G(\Omega') \) for minimum-energy states should resemble a
‘bonding’ linear-combination of s-like orbitals (i.e. an approximately gaussian \( \theta \)-dependence around the various SEMs (Eq. (28))). The coefficients \( c_{i\alpha} \) in the expression for \( G(\Omega') \) in Eq. (28) will therefore be identical for all the SEM minima \( \{ \Omega'_i \} \) corresponding to this same ring ordering. Since \( G(\Omega') \) corresponds to a linear combination of identical orbitals with the same coefficient, the overall effect of the transformation on \( G(\Omega') \) due to ring rotation will be quite small; we simply move between this subset of SEMs \( \{ \Omega'_i \} \) each of which has the same local orbitals. In contrast, the effect on the \( \theta' \) variable is relatively important; it follows from Eq. (8) that \( \theta_j \rightarrow \theta_j + \frac{2\pi}{N_m} \) corresponds to \( \theta' \rightarrow \theta' + \Delta \theta' \) where \( \Delta \theta' = N_m \frac{2\pi}{N_m(N-1)} = \frac{2\pi}{(N-1)} \). The total function \( F(\Omega) = e^{iJ\theta}G(\Omega') \) hence becomes \( e^{iJ\Delta \theta'}F(\Omega) \). Given that \( N_m \) is an even number, rotation of the \( m \)’th ring by \( \frac{2\pi}{N_m} \) necessarily corresponds to an odd number of interchanges \( i \leftrightarrow j \). If we assume the electrons are spin polarized, the spatial part of the \( N \)-electron wavefunction must be totally antisymmetric and hence the overall phase change must equal \( e^{in(2n+1)} \) where \( n \) is any integer. Denoting the \( J \) value as \( J_{WX} \) we therefore obtain the condition

\[
J_{WX} = \frac{1}{2}(N-1)(2n+1) .
\]

Importantly, this criterion for \( J_{WX} \) is independent of \( m \) and hence holds for all rings \( m \). In other words, this criterion guarantees that the \( N \)-electron wavefunction has the correct permutational symmetry under the subset of all permutations of \( N \) electrons which correspond to ring rotations. Note that \( J_{WX} \) must be an integer.

Now consider the Wigner crystal plus defect (WXD). Fisher, Halperin and Morf\textsuperscript{26} showed that the lowest energy defect states correspond to interstitial defects, i.e. an extra electron sits on an interstitial site in the otherwise perfect crystal. Single vacancies have a higher energy. Following Fisher et al., there are two types of interstitial site, ‘centered’ and ‘edge’ interstitials, and these are by far the most predominant type of defect at finite temperatures. In our model, these defects can be created by introducing an \( (N+1) \)’th electron which forms the defect. There are several reasons why this is reasonable. First, the alternative scheme of allowing one of the \( N \) existing electrons to form the defect would create an interstitial
plus vacancy; following Fisher et al. the total energy of such a defect is approximately three times larger than a single interstitial. Second, creation of such an interstitial-vacancy pair would involve a transformation of both \( \theta \) and \( \alpha \) coordinates within the \( N \)-electron \( \Omega \)-space. Third, the definition of the \( \theta_{[j]} \) variables (see Eq. (9)) is independent of the coordinates of electron \( N + 1 \). Hence the \( N \)-electron \( \Omega' \) coordinate system is essentially unchanged by the presence of the extra electron. The hyperangular function \( G(\Omega') \) for the \( N \) electron system can therefore be compared directly to the corresponding hyperangular function for the \( N + 1 \) electron system when projected onto the \( N \)-electron \( \Omega' \) space. We wish to consider the effect of this defect on ring \( m \). Following Fisher et al.\(^{26}\) the distortion of the crystal will be well-localized around the defect. In terms of the hyperangular coordinates, part of the local crystal distortion will be subsumed in the coordinate \( r \) and the effect on the hyperangles \( \alpha \) and \( \theta \) of the electrons in ring \( m \) will be relatively small unless the defect lies in ring \( m \).

Assume the defect lies in ring \( m = m_d \). The antisymmetry condition obtained above for the perfect crystal \((J_{W,\chi})\) will still be approximately valid for all rings with \( m \neq m_d \). In ring \( m_d \), there are now an odd number of electrons \( N_m + 1 \). The rotation \( \theta_j \rightarrow \theta_j + \frac{2\pi}{N_{m}+1} \) now corresponds to \( \theta' \rightarrow \theta' + \Delta \theta' \) where \( \Delta \theta' = (N_m + 1) \frac{2\pi}{(N_{m}+1)N} = \frac{2\pi}{N} \) (N.B. we now have an \((N + 1)\) electron system). Because of the odd-member ring, rotation corresponds to an even number of \( i \leftrightarrow j \) interchanges. The hyperangular function for the \( N + 1 \) electron system of crystal plus defect, when projected onto the original \( N \)-electron \( \Omega' \)-space, is essentially unchanged – the original \( N \) electrons are only slightly distorted by the presence of the defect.

Hence the overall phase change \( e^{iJ\Delta \theta'} \) must equal \( e^{i2\pi n'} \) where \( n' \) is any integer. Denoting the \( J \) value as \( J_{W,XD} \) we therefore obtain the condition

\[
J_{W,XD} = Nn'.
\]  

(30)

Again, this criterion for \( J_{W,XD} \) is independent of \( m \) and hence holds for a single defect located in any ring \( m \). Also, \( J_{W,XD} \) must be an integer. These two criteria, taken together, therefore guarantee that the \( N \)-electron wavefunction has the correct permutational symmetry under the subset of all permutations of \( N \) electrons which correspond to ring rotations, both for
the perfect crystal (WX) and the crystal plus defect (WXD). For the perfect crystal, we can consider \( N \) to be odd since each ring contains an even number of electrons, plus there is one electron at the center. Combining the two conditions for \( J_{WX} \) and \( J_{WXD} \) we hence see that the WX and WXD have the following common \( J \) values:

\[
J_m = \frac{1}{2} N(N - 1)(2n + 1)
\]  

where \( n \) is any integer. Converting these \( J_m \)-values into filling factors using the formula

\[
\nu = \frac{N(N-1)}{2J_m},
\]

which is valid for large \( N \), yields

\[
\nu = \frac{1}{2n + 1}.
\]  

This coincides with the principal series of FQHE fractions, i.e. \( \frac{1}{3} \) and \( \frac{1}{5} \). The value \( \nu = 1 \) will be discussed below. As an illustration we consider the case of \( N = 201 \) electrons. The allowed \( J_{WX} \) values are \( 100 \times 1, 100 \times 3, 100 \times 5 \) etc. while the allowed \( J_{WXD} \) values are \( 201 \times 1, 201 \times 2, 201 \times 3 \) etc. It is clear that common \( J \) values are given by \( J_m = 100 \times 201 \times 1, 100 \times 201 \times 3 \) etc. and hence \( \nu = \frac{1}{3}, \frac{1}{5} \).

### III.2 Spin-unpolarized system

We have so far generated the \( J_m \) values for a system of spin-polarized particles. Next we consider the opposite limit of a spin-unpolarized system, i.e. \( N_+ = N_- \) where \( N = N_+ + N_- \) and \( N \) must therefore be an even number. The arguments will be more approximate in this case, but we believe will still contain the essential physics. Consider a ‘typical’ ring as before. Let this ring, \( m \), contain \( N_m \) electrons where \( N_m >> 1 \): the ring will typically have \( \frac{N_m}{2} \) up-spins and \( \frac{N_m}{2} \) down-spins. Due to the Pauli principal keeping like spins apart, we will assume that on the average the ordering corresponds to the alternating sequence up-spin–down-spin repeated around the ring (See Fig. 6(a)). Rotation of the ring to a topologically identical configuration now involves a rotation of all the electrons in the ring by an angle \( \frac{2\pi}{(N_m/2)} \), i.e. we have to rotate through twice \( \frac{2\pi}{N_m} \). The rotation \( \theta_j \rightarrow \theta_j + \frac{2\pi}{(N_m/2)} \) corresponds to \( \theta' \rightarrow \theta' + \Delta\theta' \) where \( \Delta\theta' = N_m \frac{2\pi}{(N_m/2)(N-1)} = \frac{4\pi}{(N-1)} \). Since \( N_m \) is an even number, \( \frac{N_m}{2} \) can
either be odd or even. Rotation of the \( m \)'th ring by \( \frac{4\pi}{N_m} \) therefore corresponds to either an even or odd number of interchanges \( i \leftrightarrow j \) for both spin-up and spin-down electrons. Hence the total number of interchanges of like spins is always even. The overall phase change must therefore equal \( e^{i2\pi n} \) where \( n \) is any integer. Denoting the \( J \) value as \( J_{WX} \) we therefore obtain the condition

\[
J_{WX} = \frac{1}{2}(N - 1)n .
\]  

(33)

Again this criterion for \( J_{WX} \) is independent of \( m \) and hence holds for all rings \( m \). Now consider the Wigner crystal plus defect (WXD) with the defect in ring \( m \). The defect corresponds to an extra electron which can either be spin-up or spin-down. There are now an odd number of electrons \( N_m + 1 \). We now have, for large \( N_m \), that \( \Delta \theta' \approx 2(N_m + 1) \frac{2\pi}{(N_m + 1)N} = \frac{4\pi}{N} \) for the \( N + 1 \) electron system. Because of the odd-member ring, rotation now corresponds to an overall odd number of \( i \leftrightarrow j \) interchanges. This is because either the spin-up interchanges are odd while the spin-down are even, or vice versa. Hence the overall phase change \( e^{iJ\Delta \theta'} \) must equal \( e^{i\pi(n' + 1)} \) where \( n' \) is any integer. Denoting the \( J \) value as \( J_{WXD} \) we therefore obtain the condition

\[
J_{WXD} = \frac{1}{2}N(n' + \frac{1}{2}) .
\]  

(34)

Again, this criterion for \( J_{WXD} \) is independent of \( m \). These two criteria, taken together, therefore guarantee that the spin-unpolarized \( N \)-electron wavefunction has the correct permutational symmetry under the subset of all permutations of \( N \) electrons which correspond to ring rotations, both for the perfect crystal (WX) and the crystal plus defect (WXD). Combining the two conditions for integer values of \( J_{WX} \) and \( J_{WXD} \) we hence see that the WX and WXD have the following common \( J \) values:

\[
J_m = \frac{1}{4}N(N - 1)(2n + 1)
\]  

(35)

where \( n \) is any integer. Converting these \( J_m \) values into filling factors yields

\[
\nu = \frac{2}{2n + 1} .
\]  

(36)
This coincides with the second series of FQHE fractions, i.e. $\frac{2}{3}, \frac{4}{5}, \frac{2}{7}$ etc. and hence suggests that the ground states at these fractions will be spin-unpolarized in the absence of Zeeman energy, in agreement with earlier finite-size numerical calculations (see p. 63 of Ref. 3). Interestingly the series also reproduces the IQHE value $\nu = 2$. As an illustration we consider the case of $N = 200$ electrons. The allowed $J_{WX}$ values are $199 \times 1$, $199 \times 2$, $199 \times 3$ etc. while the allowed $J_{WXD}$ values are $50 \times 1$, $50 \times 3$, $50 \times 5$ etc. Common $J$ values are given by $J_m = 199 \times 50 \times 1$, $199 \times 50 \times 3$ etc. and hence $\nu = \frac{2}{3}, \frac{2}{5}$ etc.

### III.3 Partially spin-polarized system

Consider a partially spin-polarized system. First we will take i.e. $N_+ = 3N_-$ where $N = N_+ + N_-$ and $N$ is again even. Consider a ‘typical’ ring as before. Let this ring, $m$, contain $N_m$ electrons where $N_m >> 1$: the ring will typically have $\frac{3N_m}{4}$ up-spins and $\frac{N_m}{4}$ down-spins. Due to the Pauli principal keeping like spins apart, we will now assume that on the average the ordering corresponds to the sequence up-spin–up-spin–up-spin–down-spin repeated around the ring (see Fig. 6(c)). Rotation of the ring to a topologically identical configuration now involves a rotation of all the electrons in the ring by an angle $\frac{2\pi}{N_m/4}$, i.e. we have to rotate through four times $\frac{2\pi}{N_m}$. The rotation $\theta_j \rightarrow \theta_j + \frac{2\pi}{N_m/4}$ corresponds to $\theta' \rightarrow \theta' + \Delta \theta'$ where $\Delta \theta' = N_m\frac{2\pi}{N_m/4(N-1)} = \frac{8\pi}{N-1}$. Since $N_m$ is an even number, $\frac{3N_m}{4}$ and $\frac{N_m}{4}$ are either both odd or both even. Rotation of the $m$th ring by $\frac{8\pi}{N_m}$ therefore corresponds to either an even or odd number of interchanges $i \leftrightarrow j$ for both spin-up and spin-down electrons. Hence the total number of interchanges of like spins is always even. The overall phase change must therefore equal $e^{2\pi n}$ where $n$ is any integer. Denoting the $J$ value as $J_{WX}$ we therefore obtain the condition

$$J_{WX} = \frac{1}{4}(N-1)n . \tag{37}$$

Again this criterion for $J_{WX}$ is independent of $m$ and hence holds for all rings $m$. Now consider the Wigner crystal plus defect (WXD) with the defect in ring $m$. The defect can either be spin-up or spin-down. There are now an odd number of electrons $N_m + 1$. We
now have, for large $N_m$, that $\Delta \theta' \approx 4(N_m + 1) \frac{2\pi}{(N_m + 1)N} = \frac{8\pi}{N}$ for the $N + 1$ electron system. Because of the odd-member ring, rotation now corresponds to an overall odd number of $i \leftrightarrow j$ interchanges. This is because either the spin-up interchanges are odd while the spin-down are even, or vice versa. Hence the overall phase change $e^{iJ \Delta \theta'}$ must equal $e^{i\pi(2n'+1)}$ where $n'$ is any integer. Denoting the $J$ value as $J_{WXD}$ we therefore obtain the condition

$$J_{WXD} = \frac{1}{4} N(n' + \frac{1}{2}).$$  

(38)

Again, this criterion for $J_{WXD}$ is independent of $m$. These two criteria, taken together, therefore guarantee that the partially spin-polarized $N$-electron wavefunction has the correct permutational symmetry under the subset of all permutations of $N$ electrons which correspond to ring rotations, both for the perfect crystal (WX) and the crystal plus defect (WXD). Combining the two conditions for integer values of $J_{WX}$ and $J_{WXD}$ we hence see that the WX and WXD have the following common $J$ values:

$$J_m = \frac{1}{8} N(N - 1)(2n + 1)$$  

(39)

where $n$ is any integer. Converting these $J_m$-values into filling factors yields

$$\nu = \frac{4}{2n + 1}.$$  

(40)

This coincides with the fourth series of FQHE fractions, i.e. $\frac{4}{5}, \frac{4}{7}$ etc., hence the theory suggests that the corresponding ground states at these fractions will be partially spin-polarized in the ratio of spin-up to spin-down of 3 : 1 in the absence of Zeeman energy. Again this is in agreement with finite-size numerical calculations (see p. 63 of Ref. 3). As an illustration we again consider the case of $N = 200$ electrons (N.B. we have 4 as a factor since the ratio of spin-up to spin-down is 3 : 1). The allowed $J_{WX}$ values are $199 \times 1, 199 \times 2, 199 \times 3$ etc. while the allowed $J_{WXD}$ values are $25 \times 1, 25 \times 3, 25 \times 5$ etc. Common $J$ values are given by $J_m = 199 \times 25 \times 1, 199 \times 25 \times 3$ etc. and hence $\nu = \frac{4}{5}, \frac{4}{7}$ etc.

Next we take i.e. $N_+ = 2N_-$ where $N = N_+ + N_-$ and $N$ is again even. Consider a ‘typical’ ring as before. Let this ring, $m$, contain $N_m$ electrons where $N_m >> 1$: the ring
will typically have \( \frac{2N_m}{3} \) up-spins and \( \frac{N_m}{3} \) down-spins. Due to the Pauli principal keeping like spins apart, we will assume that on the average the sequence corresponds to up-spin–up-spin–down-spin repeated around the ring (see Fig. 6(b)). Rotation of the ring to a topologically identical configuration now involves a rotation of all the electrons in the ring by an angle \( \frac{2\pi}{(N_m/3)} \), i.e. we have to rotate through three times \( \frac{2\pi}{N_m} \). The rotation \( \theta_j \rightarrow \theta_j + \frac{2\pi}{(N_m/3)} \) corresponds to \( \theta' \rightarrow \theta' + \Delta \theta' \) where \( \Delta \theta' = N_m \frac{2\pi}{(N_m/3)(N-1)} = \frac{6\pi}{(N-1)} \). Since \( N_m \) is an even number, \( \frac{2N_m}{3} \) and \( \frac{N_m}{3} \) are either both odd or both even. Rotation of the \( m \)'th ring by \( \frac{6\pi}{N_m} \) therefore corresponds to either an even or odd number of interchanges \( i \leftrightarrow j \) for both spin-up and spin-down electrons. Hence the total number of interchanges of like spins is always even. The overall phase change must therefore equal \( e^{i2\pi n} \) where \( n \) is any integer. Denoting the \( J \) value as \( J_{WX} \) we therefore obtain the condition

\[
J_{WX} = \frac{1}{3}(N - 1)n.
\] (41)

Again this criterion for \( J_{WX} \) is independent of \( m \) and hence holds for all rings \( m \). Now consider the Wigner crystal plus defect (WXD) with the defect in ring \( m \). The defect can either be spin-up or spin-down. There are now an odd number of electrons \( N_m + 1 \). We now have, for large \( N_m \), that \( \Delta \theta' \approx 3(N_m + 1)\frac{2\pi}{(N_m + 1)N} = \frac{6\pi}{N} \) for the \( N + 1 \) electron system.

Because of the odd-member ring, rotation now corresponds to an overall odd number of \( i \leftrightarrow j \) interchanges. This is because either the spin-up interchanges are odd while the spin-down are even, or vice versa. Hence the overall phase change \( e^{iJ\Delta \theta'} \) must equal \( e^{in(2n'+1)} \) where \( n' \) is any integer. Denoting the \( J \) value as \( J_{WXD} \) we therefore obtain the condition

\[
J_{WXD} = \frac{1}{3}N(n' + \frac{1}{2}).
\] (42)

Again, this criterion for \( J_{WXD} \) in independent of \( m \). These two criteria, taken together, therefore guarantee that the partially spin-polarized \( N \)-electron wavefunction has the correct permutational symmetry under the subset of all permutations of \( N \) electrons which correspond to ring rotations, both for the perfect crystal (WX) and the crystal plus defect (WXD). Combining the two conditions for integer values of \( J_{WX} \) and \( J_{WXD} \) we hence see that the WX and WXD have the following common \( J \) values:
\[ J_m = \frac{1}{6} N(N - 1)(2n + 1) \]  

(43)

where \( n \) is any integer. Converting these \( J_m \) values into filling factors yields

\[ \nu = \frac{3}{2n + 1}. \]

(44)

This coincides with the third series of FQHE fractions, i.e. \( \frac{3}{5}, \frac{5}{7} \text{ etc.} \) and predicts the corresponding ground states to be partially spin-polarized in the ratio of spin-up to spin-down of 2 : 1 (or vice versa) in the absence of Zeeman energy. We note that there is an alternative system that also yields the filling factor series \( \nu = \frac{3}{2n+1} \). In particular, this fraction emerges from considering a fully spin-polarized system but now considering rotation of two rings simultaneously. These two states with \( N_+ : N_- = 2 : 1 \) and \( N_- = 0 \) respectively, probably compete to become the ground-state depending on the value of the Zeeman energy (and hence magnetic field). Interestingly, finite-size studies have shown that the \( \nu = \frac{3}{5} \) state is indeed partially polarized for \( B < 15T \) in the ratio \( N_+ : N_- = 2 : 1 \) but fully polarized for \( B > 15T \) (see p.160 of Ref. 3).

The above arguments can be extended straightforwardly to consider \( N_+ = (p - 1)N_- \) where \( N = N_+ + N_- \) and \( p \) is any integer. In this case, the corresponding filling fraction becomes \( \nu = \frac{p}{2n+1} \). We now focus on the filling factor \( \nu = 1 \) (IQHE). We have already shown that this state emerges from the two following series: \( \nu = \frac{1}{2n+1} \) for \( n = 0 \) in a fully spin-polarized system, or \( \nu = \frac{3}{2n+1} \) for \( n = 1 \) in a partially spin-polarized system. In fact for a given spin polarization \( N_+ = (p - 1)N_- \) with \( p \) odd, the factor \( \nu = 1 \) will always arise, i.e. by choosing \( n = \frac{p-1}{2} \). It is reasonable to expect these states to compete to become the ground-state. This is consistent with recent findings that a gap exists at \( \nu = 1 \) (IQHE) even in the absence of Zeeman splitting. The possible coexistence of a manifold of partially spin-polarized states is also consistent with the idea of macroscopic spin-textures near \( \nu = 1 \); in particular, taking a linear combination of partially spin-polarized states enables the construction of localized ‘wave-packets’ of spin – we conjecture that the resulting spin-textures may be related to skyrmions.
We note that the above filling factors emerged from requiring that the WX and WXD had a common angular momentum value. The defect was considered to be an interstitial electron. It turns out that, as far as the common \( J_m \) values are concerned, we could also have considered the defect to be a vacancy. The product \((N-1)(N-2)\) would have appeared throughout this section instead of \(N(N-1)\); in the large \(N\) limit, both products yield \(\sim N^2\) and hence the same filling factors. Hence at \(J = J_m\), the WX can coexist with a WXD where the defect is either an interstitial electron or a vacancy. As noted earlier, however, such vacancies do have a higher energy and hence are less likely to occur at finite temperatures.

**IV. ANALYTIC CALCULATION OF FQHE ENERGY GAPS**

In this section we will give an analytic calculation for the energy gaps associated with the FQHE and IQHE states, i.e. for \(J = J_m\). The calculation is approximate since it relies on the various approximations made in Sec. II.3. However our goal is to find whether the gaps predicted by our model are in fact consistent with the observed FQHE gaps and also to identify trends in the energy gaps with filling fraction, magnetic field etc.

In Sec. II.3 we obtained an approximate expression for the relative energy \(E_{\text{rel}}\) (see Eq. (27)). This energy depends on \(E_\alpha\) and \(E_\theta\). In Sec. III we argued that the important criterion characterising the magic-number \(J\)-values was that the crystal (WX) and defect (WXD) can both have the same \(J\) value given by \(J = J_m\); this leads to a large delocalization energy due to increased WX-WXD tunnelling in \(\Omega'\)-space. In the language of single-particle tight-binding theory, the resulting energy gap between states with \(J = J_m\) and \(J \neq J_m\) arises from the hybridization of the \(G(\Omega')\) solutions peaked around, for example, \(\Omega'_0\) and \(\Omega'_{0,\alpha}\) at \(J = J_m\). This hybridization hence yields a low \(E_{\text{rel}}\) because of the corresponding delocalization of \(G(\Omega')\) at \(J = J_m\), i.e. a reduction in zero-point energy. Here we will obtain an analytic expression for this energy using a simple model for the effect of delocalization and show that the resulting gaps are consistent with experimental findings.

As pointed out earlier, a state of a given negative \(J\) will have an energy minimum at
a finite magnetic field $\omega_c$. As $\omega_c$ increases, the value of $J$ at which the energy $E_{\text{rel}}(J)$ has a minimum will increase. We will calculate the energy difference between a state with $J = J_m$ and competing low-energy states with $J$ given by $J_{m\pm} = J_m \pm \delta$ at a given $\omega_c$, where $\delta \ll J_m$. The lowest energy state with $J = J_m$ is given by Eq. (27) with $n = 0$:

$$E_{\text{rel}}(J_m) = \hbar \omega_0(B)\left((N-2)^2 + J_m^2 + \frac{2m^*\beta}{\hbar^2} V(\Omega'_0) + \frac{2m^*}{\hbar^2} [E_\theta(J_m) + E_\alpha(J_m)]\right)^{\frac{1}{2}} + 1 - J_m \frac{\hbar \omega_c}{2}$$

(45)

while that with $J = J_{m\pm}$ is given by:

$$E_{\text{rel}}(J_{m\pm}) = \hbar \omega_0(B)\left((N-2)^2 + [J_m \pm \delta]^2 + \frac{2m^*\beta}{\hbar^2} V(\Omega'_0) + \frac{2m^*}{\hbar^2} [E_\theta(J_{m\pm}) + E_\alpha(J_{m\pm})]\right)^{\frac{1}{2}} + 1 - [J_m \pm \delta] \frac{\hbar \omega_c}{2}.$$  

(46)

As discussed in Sec. II.1, the angular momentum is negative for low-lying energy states, hence we have included the minus sign directly into these expressions, i.e. $J_m$ and $J_{m\pm}$ are positive numbers. Consider the state with $J = J_m$. This state can coexist as both a crystal (WX) and a crystal plus defect (WXD), in contrast to the state $J_{m\pm}$. The transition WX → WXD will involve a distortion of the $\Omega'$-coordinates. This distortion in $\Omega'$-space corresponds to a spreading or ‘delocalization’ of the function $G(\Omega')$ along these directions. There is therefore a reduction in ‘localization’ energy going from a state with $J \neq J_m$ (i.e. WX and WXD cannot coexist) to a state with $J = J_m$ (i.e. WX and WXD can coexist). We will hence write:

$$E_\theta(J_m) + E_\alpha(J_m) + \beta V(\Omega'_0) = E_0$$

(47)

while

$$E_\theta(J_{m\pm}) + E_\alpha(J_{m\pm}) + \beta V(\Omega'_0) = E_0 + \tilde{\Delta}$$

(48)

where $\tilde{\Delta}$ represents the increased localization energy of state $J_{m\pm}$ as compared to $J_m$. Note that the potential energy minimum $\beta V(\Omega'_0)$ is a constant term throughout. In the Appendix we show that typically $\tilde{\Delta} \sim N^2$ while $E_0 \sim N^3$. Hence in the limit of $N \gg 1$, we have
We are interested in the large $N$ limit since our goal is to calculate the FQHE gaps: hence we will choose the confinement $\omega_0 << \omega_c$ which yields $\omega_0(B) \sim \frac{\omega_c}{2}$. Let us first consider the filling factor $\nu = \frac{1}{3}$ hence $J_m = 3\frac{N(N-1)}{2}$. Substituting into Eq. (49) we obtain the approximate expression for the energy gap

$$\Delta E_{\frac{1}{3}} \sim \frac{1}{3} \frac{m^* \tilde{\Delta}}{N^2 \hbar^2} \hbar \omega_c.$$  

There are several points to note about this expression for the energy gap at $\nu = \frac{1}{3}$.

(i) Given that $\tilde{\Delta} \sim N^2$ for large $N$, the expression is independent of the electron number $N$. It is also independent of the strength of the parabolic potential $\omega_0$. For a given $\omega_c$ corresponding to the filling factor $\nu = \frac{1}{3}$, we can therefore take the thermodynamic limit $N \to \infty$ and yet still maintain a fixed average electron density by choosing appropriately small values of $\omega_0$. Our expression for the energy gap at filling factor $\nu = \frac{1}{3}$ which was derived in terms of $J$ values for a fixed-$N$ system therefore also holds for an infinite two-dimensional electron gas of fixed density.

(ii) The expression for the energy gap does not exhibit a direct dependence on the value of the electron-electron interaction $\beta$. We do emphasize, however, that throughout most of this paper we have assumed that $\beta$ is large enough to be able to neglect tunnelling between SEMs. Hence we can only conclude that the absolute value of $\beta$ does not directly affect the energy gap $\Delta E$ for sufficiently large $\beta$. This is consistent with experimental findings that the gap can be remarkably sample-independent. Below we will mention how a weak dependence on $\beta$ will arise if one considers smaller values of $\beta$.

(iii) The energy gap appears to be approximately linear in the magnetic field. Most previous theoretical studies conclude that the dependence resembles $B^{\frac{1}{2}}$. As we will show below, the linear dependence is in reasonable agreement with experimental data, particularly at lower
fields. However, we will later discuss how a weaker, non-linear dependence, i.e. $B^x$ where $x < 1$, can eventually arise at larger $B$ in our model.

(iv) The energy gap does not depend on $\delta$ to first order in $(\frac{\delta}{j_m})$. This independence of $\delta$ is important since it implies that the energy gap exists between state $J_m$ and all other states with $J$ in the vicinity of $J_m$. We know from the discussion at the end of Sec. II.1 that, over a given range of magnetic field, the states which compete to become the ground state will be those of similar $J$. Hence we expect the energy gap arising to exist over a small but finite range of magnetic field, as observed experimentally.

(v) The expression for the gap $\Delta E$ can be made applicable to situations where the lowest-energy excitation involves spin-flips, by adding $\Delta E_{\text{spin}}$ where $\Delta E_{\text{spin}}$ is the difference in total spin energy between the excited state and the $\nu = \frac{1}{3}$ spin-polarized ground state. However, we are interested in the lowest-energy excitations, and hence will take $\Delta E_{\text{spin}} = 0$ since $\Delta E_{\text{spin}} \geq 0$ for the fully spin-polarized initial state at $\nu = \frac{1}{3}$. For other fractions, the term $\tilde{\Delta}$ will have an indirect dependence on the spin configuration since, for a mixed spin system, the $\Omega'$ space is really coupled to the spinor space by the antisymmetry condition, hence $G'(\Omega')$ is actually a two-dimensional vector. A detailed discussion of spin-reversed excited states will be given elsewhere.

(vi) Given the discussion in (v), together with the fact that $\tilde{\Delta}$ has a weak but finite dependence on $J_m$ (see later), we can conclude the value of $\tilde{\Delta}$ will generally be different for different fractions. Gaps at other fractions in the $\nu = \frac{p}{3}$ series are discussed below.

We will now attempt to derive an approximate analytic expression for $\tilde{\Delta}$. Consider the $N$-electron system at $J = J_m$. As discussed in Sec. III, the system can exist as both a crystal (WX) and a crystal plus defect (WXD), in contrast to the state $J_{m\pm}$. We will argue in what follows that the transition WX$\rightarrow$WXD involves a significant fractional distortion of $\theta$-coordinates. This distortion along the $\{\theta_{[j]}\}$-axes in $\Omega'$-space corresponds to a spreading or ‘delocalization’ of the function $G'(\Omega')$ along these directions, thereby giving rise to a finite $\tilde{\Delta}$. In Secs. II and III, we argued that the low-energy SIMs near a given SEM consisted of a single electron defect placed at an interstitial site within the hexagonal
crystal. As noted at the end of Sec. III the defect could also be a vacancy, although the corresponding SIM would have a higher energy. Consider a defect placed in ring \( m \) which contains \( N_m \) particles with \( N_m >> 1 \), and let the defect be sited between \( j \) and \( j+1 \) (c.f. Fig. 5). Classically, the system moves to a nearby SIM in \( \Omega' \)-space (c.f. Fig. 2). In particular the defect will cause a distortion of the coordinates of particle \( j \). In order to calculate the maximum possible distortion (and hence delocalization available as a result of the hybridization between the SEM and SIM) we will consider the particular SIM in which only particle \( j \) moves to accomodate the defect. In principle, both the \( \alpha_j \) and \( \theta[j] \) coordinates will be modified, thereby ‘sharing’ the effect of the distortion. However, with the defect placed between \( j \) and \( j+1 \) in ring \( m \), the distortion of particle \( j \) will mainly be along the \( \theta[j] \) direction. The idea that the most important effect of the defect is the distortion of the \( \theta \)-coordinates, is consistent with the following considerations. Consider any particle \( j' \) nearby to the defect with coordinates \( \theta[j'] \) and \( \alpha[j'] \). Let the nearby defect cause a distortion of \( a \) in all directions. Hence the new coordinates of the particle \( j' \) are approximately \( \alpha[j'] + a \) and \( \theta[j'] + \frac{a}{\alpha[j']} \). The relative distortion caused by the nearby defect is hence \( \frac{\Delta \alpha[j']}{\alpha[j']} \sim \frac{a}{\alpha[j']} \) while \( \frac{\Delta \theta[j']}{\theta[j']} \sim \frac{a}{\alpha[j'] \theta[j']} \). For \( N >> j' \), \( \alpha[j'] \) changes slowly with \( j' \) and is unchanged if \( j' \) lies in ring \( m \). However \( \theta[j'] \) ranges from 0 to \( 2\pi \) within ring \( m \) and hence the fractional change \( \Delta \theta[j'] \) can be significant.

We will therefore consider \( \bar{\Delta} \) as arising as a result of the difference in \( E_\theta \) for \( J_m \) as compared to \( J_{m\pm} \). The loss of ‘localization’ energy of the state \( J_m \) as compared to \( J_{m\pm} \) can be significant along the \( \{\theta[j]\} \)-directions, i.e. \( E_\theta \) can differ appreciably depending on whether the function \( G(\Omega') \) is localized (i.e. \( J = J_{m\pm} \)) or not (\( J = J_m \)). Consider Eq. (26) for the ‘energy’ \( e_j \) associated with a particle \( j \) in ring \( m \) where \( J \neq J_m \) (i.e. WX and WXD cannot coexist). The equation resembles a one-dimensional Schrodinger equation in \( \theta[j] \) for a mass \( \alpha[j_0] \) moving in a potential \( w_j(\theta[j] - \theta[j_0]) \). The function \( w_j \) will have a minimum at \( \theta[j] = \theta[j_0] \), whereas there are maxima at \( \theta[j] = \theta[j_0] \pm \frac{2\pi}{N_m} \) as particle \( j \) approaches particle \( j \pm 1 \).
produced a minimum at $y = 0$ and maxima at $y = \pm \frac{\pi}{2}$. We can approximate $e_j$ using a simple one-dimensional particle-in-a-box model: we will assume that $w_j$ is a flat-bottomed potential with infinite walls at $\theta_j = \theta_{j0} \pm \frac{2\pi}{N_m}$. The width of the box is therefore given by $a_j = \frac{4\pi}{N_m}$. The energy $e_j^{(J)}$ is hence approximately given by

$$e_j^{(J)} \sim \frac{\hbar^2 \pi^2 N_m^2}{2m^2 \alpha_j^2 [4\pi]^2}.$$  \hspace{1cm} (51)

Note that the width of the wavefunction $g_j$, and hence the localization of $G(\Omega')$ along $\theta_j$, is characterized by $a_j$. This expression (Eq. (51)) for $e_j^{(J)}$ implicitly assumes that the electron-electron interaction $\beta$ is large; for smaller values of $\beta$, the particle-in-a-box energy should pick up a weak dependence on $\beta$. Throughout this paper, however, we will use the approximate analytic form given in Eq. (51). At $J = J_m$ there is distortion of $G(\Omega')$ since WX and WXD can coexist. The defect can occupy any interstitial site in the crystal; each defect position produces a distinct SIM. There exists a SIM (e.g. $\Omega'_{0,j}$) in which the defect is placed next to particle $j$, say between particles $j$ and $j + 1$ as used earlier. We can see that there is one such SIM associated with each $\theta_j$ coordinate. If, as discussed above, we consider the main distortion as occurring on the $\theta_j$ coordinate of particle $j$, then the associated SIM lies on the $\theta_j$ axis. In this case the coexistence of the SEM $\Omega'_0$ and the SIM $\Omega'_{0,j}$ causes an increase in the effective box-width, $a_j \rightarrow a_j + \delta a_j$. The energy along the $\theta_j$ direction is now given by

$$e_j^{(J_m)} \sim e_j^{(J)} + \frac{\partial e_j^{(J)}}{\partial a_j} \delta a_j \sim e_j^{(J)} [1 - 2 \frac{\delta a_j}{a_j}].$$  \hspace{1cm} (52)

Although there are many such SIMs associated with each SEM, we know that the defects have a low density at the temperatures of interest. The system also requires a large time to tunnel between these SIMs since each SIM describes a different defect position in the crystal: diffusion of the defect between sites will be slow at low temperatures. It is reasonable therefore to suppose that each SEM hybridizes with just one of these SIMs at any time. The average loss of localization energy of state $J_m$ as a result of distortion due to a nearby SIM is therefore obtained by averaging over all $(N - 2) \theta_j$ coordinates. Hence using Eq. (52)
\[ \tilde{\Delta} \sim \frac{1}{N-2} \sum_j 2[\delta a_j]e_j^{(J)} \sim 2[\overline{\delta a}] \bar{e} \]  
\text{(53)}

where \( \bar{x} \) represents an average of the quantity \( x \) over all \((N-2)\) of the \( \theta_{[j]} \) coordinates.

We could also try to obtain expressions for \( \Delta E \) at other fractions. Consider \( \nu = \frac{1}{5} \). Equation (50) now has the factor \( \frac{1}{3} \) replaced by \( \frac{1}{5} \). Assuming as a crude approximation that the values of \( \tilde{\Delta} \) are the same, we obtain the result that \( \Delta E_{\frac{1}{5}} : \Delta E_{\frac{1}{3}} \sim 0.6 \) for samples at a given magnetic field. The literature tends to put this ratio at about \( 0.3-0.4 \). One could also try to evaluate \( \Delta E \) for other fractions where the ground-state \( J_{m} \) and/or the excited states \( J_{m\pm} \) are thought to have spin-reversed electrons. Such a calculation needs a more careful estimation of \( \tilde{\Delta} \), as discussed earlier. Here we will just provide a rough estimate by considering, as before, excitations which do not change the total spin component (i.e. \( \Delta E_{\text{spin}} = 0 \)). We will choose \( \nu = \frac{2}{3} \) in order to compare with the results for \( \nu = \frac{1}{3} \). There are two effects of considering \( \nu = \frac{2}{3} \) instead of \( \nu = \frac{1}{3} \) when re-deriving the expressions obtained in this section. The prefactor in Equation (50) increases by a factor of 2, while \( \frac{\delta a_j}{a_j} \) decreases by a factor of 2. This decrease in \( \frac{\delta a_j}{a_j} \) arises as follows. Recall that like spins in the spin unpolarized case are separated by twice the angle of the spin-polarized case. The ‘unit-cell’ size in \( \Omega’ \)-space is determined by the separation between neighboring SEMs, and is therefore twice as large for the unpolarized case. The effective box size must therefore also be twice as large, i.e. the effective \( a_j \) value is now \( \frac{8\pi}{Nm} \) instead of \( \frac{4\pi}{Nm} \). Hence the final result is that \( \Delta E_{\frac{2}{3}} \sim \Delta E_{\frac{1}{3}} \). Although we do not attach too much importance to this result because of the complications of spin, it is interesting to note that experimentally the gaps for \( \nu = \frac{1}{3} \) and \( \nu = \frac{2}{3} \) are found to be similar,\(^{27,28}\) as will be shown below. We note that allowing for spin-flip excitations at \( \nu = \frac{2}{3} \) may reduce the overall gap at low \( B \) since \( \Delta E_{\text{spin}} \) can be negative if the ground state is not fully spin-polarized. Hence the total gap may be negligible for \( \nu = \frac{2}{3} \) at low \( B \). This feature is also seen experimentally. The same argument concerning effective box size should also be approximately true for the other partially spin-polarized fractions in the \( \frac{p}{3} \) series. Consider \( \nu = \frac{p}{3} \). The prefactor in Equation (50) increases by a factor \( p \), while the effective box-size also increases by the same factor. The net effect is that the expression...
for the gap is similar for all fractions $\frac{p}{3}$ where $p = 1, 2, 4, 5$ etc. Hence the energy gaps for the $\frac{p}{3}$ fractions measured across a range of samples should all fall on approximately the same curve as a function of magnetic field.

Equation (53) presented an analytic expression for $\tilde{\Delta}$ which, to the level of approximation employed, did not depend on the ground state $J_m$ value. Examination of the more accurate versions of the hyperangular equation presented in Sec. II.3, suggests that $\tilde{\Delta}$ should actually have a weak but finite dependence on $J_m$ (recall, for example, Eq. (23) or (24)). In the $N = 3$ study in Sec. II.2, we found that increasing $J$ did indeed increase the localization of $G(\Omega')$ around the classical minima. For large $N$, as discussed in Sec. II.3, the dependence on $J_m$ should be weaker; however the resulting hybridization between a given SEM (i.e. WX) and nearest-neighbor SIMs (i.e. WXD) should also decrease slightly as $J_m$ increases. Decreasing hybridization will reduce the value of $\tilde{\Delta}$ as $J_m$ increases. It is interesting to analyze the effect of this reduction in $\tilde{\Delta}$ for the separate situations of (a) a given sample over a range of $\nu$ values, and (b) different samples at a given fixed $\nu$. In case (a), the number of electrons $N$ is fixed. As the value of $J_m$ increases, the value of $\omega_c$ at which this $J_m$ value represents the ground state must also increase. If $\tilde{\Delta}$ decreases as $J_m$ increases, then $\tilde{\Delta}$ must also decrease with increasing $\omega_c$. This reduction in $\tilde{\Delta}$ as $\omega_c$ increases, if sufficiently large, will make $\Delta E \rightarrow 0$: we suggest that this may be related to the predicted formation of a Wigner solid (i.e. gapless excitations) at very high magnetic fields. In case (b), fixed $\nu$ means that increasing $J_m$ requires an increase in $N$ (recall that $J_m = \frac{N(N-1)}{2\nu}$). If $\tilde{\Delta}$ decreases as $J_m$ increases, then $\tilde{\Delta}$ must also decrease as $N$ increases. However, a fixed value of $\nu$ means that increasing $N$ requires an increase in magnetic field. Hence $\tilde{\Delta}$ decreases as $\omega_c$ increases. As mentioned earlier, this will tend to weaken the linear magnetic field-dependence of the theoretical gaps at fixed $\nu$ to $\omega_c^x$ with $0 < x < 1$. Such a sub-linear dependence is consistent with recent experimental data at high fields. In the estimates of the gap discussed below, however, we take as a first approximation the form of $\tilde{\Delta}$ presented in Eq. (53). Consequently the calculated gaps for a given $\nu$ always increase linearly with magnetic field.
We now proceed to discuss appropriate values of $\frac{\delta a}{a}$ and hence calculate the gaps. The precise value for $\frac{\delta a}{a}$ will depend on the details of the crystal plus defect system (WXD). Here we will suggest reasonable lower and upper estimates, and argue that the particular value to be used will depend on the degree of disorder in the experimental samples. In particular, we will argue that the lower estimate is appropriate for disordered (i.e. lower mobility) samples while the upper estimate is appropriate for pure (i.e. higher mobility) samples.

First we consider the lower estimate for $\frac{\delta a}{a}$. Fisher et al. found that the maximum distortion for a vacancy defect was about 12%, but that the value for the interstitial defect was ‘considerably larger’. If the sample contains a significant impurity concentration, it is likely that interstitial electrons will have difficulty in diffusing through the $N$-electron system. The function $G(\Omega')$ will therefore have a restricted delocalization for kinetic reasons. In the absence of interstitial defects, the delocalization would be determined solely by the vacancies. We will therefore take the value of 12% as a lower estimated bound for $\frac{\delta a}{a}$. From the Appendix we have that $\bar{e} \sim 27\hbar^2N^2/16m^*\pi^2$ and hence $\tilde{\Delta} \sim 0.4\hbar^2N^2/m^*\pi^2$. Substituting this into the expression for the energy gap, we obtain $\Delta E_1 \sim 0.014\hbar\omega_c$ meV and hence $\Delta E_{\frac{1}{3}} \sim 0.16\hbar\omega_c$ Kelvin. Given that $1\text{meV} \equiv 1.728B[T]$ (Tesla) for GaAs, we obtain $\Delta E_{\frac{1}{3}} \sim 0.27B[T]$ Kelvin. Hence at $B = 20T$, $\Delta E_{\frac{1}{3}} \sim 5.5$ Kelvin. Figure 7 compares this lower estimated bound of the energy gap at $\nu = \frac{1}{3}$ (and hence $\nu = \frac{2}{3}$ as explained above) with early experimental results obtained by Boebinger et al. over a range of relatively impure samples (i.e. significant impurity concentration). The agreement is surprisingly good; however we emphasize that our calculation is obviously fairly crude. Apart from improving the expression for $\Delta E_{\frac{1}{3}}$ given in Eq. (50), one could do a better job in calculating the localization energy $\tilde{\Delta}$ from Eq. (53). Such improvements would almost certainly render the calculation of energy gaps within the present model numerical, although such calculations would be more straightforward than the original alternative of an $N$-electron diagonalization. Various numerical improvements will be presented in a future publication; the goal of the present paper is to pursue a purely
analytical theory.

Now we turn to an upper estimate for $\delta a/a$. We assume that the sample is pure and hence there is no kinetic reason for ignoring interstitial defects. We first recall our physical picture of the topology of the interstitial defect, stated earlier in this section. We consider a ring $m$ containing $N_m$ electrons, including particles $j - 1$, $j$ and $j + 1$ (c.f. Fig. 5). The angle between particle $j$ and $j + 1$ is $\frac{2\pi}{N_m}$, and the angle between particle $j - 1$ and $j + 1$ is $\frac{4\pi}{N_m}$. We let the defect lie in the ring between particles $j$ and $j + 1$. We are looking for an upper estimate on the value of $\delta a/a$, hence we will assume that the only particle which moves to accommodate the extra electron is particle $j$. As before, the angle between $j - 1$ and $j + 1$ is still $\frac{4\pi}{N_m}$, but now there are two particles ($j$ and the defect) within this angular range. In an equilibrium state (i.e. a SIM) the three angles between $j - 1$ and $j$, $j$ and the defect, and the defect and $j + 1$, are all equal to $\frac{4\pi}{3N_m}$. The distortion of the effective box size for particle $j$ will be determined by the angle between $j$ and $j + 1$. Hence an estimate of the average distortion $\bar{\delta a/a}$ is $\frac{2\pi}{N_m}(\frac{1}{3} - 1)$ divided by $\frac{2\pi}{N_m}$, which gives $\frac{1}{3}$. Our upper estimated value of $\bar{\delta a/a}$ is therefore 0.33. Figure 8 compares both this upper bound and the lower bound obtained earlier to experimental data obtained by the Oxford and AT&T groups for a range of relatively pure, high mobility samples. The experimental values lie between the two bounds. This consistency between the present theoretical results and experiment lends support to our interpretation of the effect of sample purity.

V. CONCLUSIONS

A microscopic theory describing a confined $N$-electron gas in two dimensions subject to an external magnetic field, was presented. The number of electrons $N$ and strength of the electron-electron interaction can be arbitrarily large. For any value of the magnetic field $B$, the correlated $N$-electron states were shown to be determined by the solution to a universal effective problem: this problem resembles that of a fictitious particle moving in a multidimensional space, without a magnetic field, occupied by potential minima corresponding to the classical $N$-electron equilibrium configurations.
A possible connection with the Fractional (FQHE) and Integer (IQHE) Quantum Hall effects was subsequently proposed. In particular, it was shown that low-energy minima can arise in the large $N$ limit at filling factors $\nu = \frac{p}{2n+1}$ where $p$ and $n$ are any positive integers. The energy gaps calculated analytically at $\nu = \frac{2}{3}$ were found to be consistent with experimental data as a function of magnetic field, over a range of samples. Various other known features of FQHE and IQHE states were found to emerge from the present theory.

While it is obviously extremely difficult to calculate many-particle energy gaps etc. accurately using an analytic approach, we hope that the general qualitative trends and orders of magnitude provided by the model will be useful in understanding the fascinating but complex field of highly-correlated $N$-electron systems. We also hope that the model may begin to shed some light on the connection between the two limits of few-electron correlated states in quantum dots, and the infinite two-dimensional electron gas.

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First we derive an approximate expression for $\bar{e}$ and hence $\tilde{\Delta}$. The exact hyperangular identity $\sum_{j=2}^{N} [\hat{\Sigma} \hat{r}]^2 = 1$ implies $\sum \alpha_j^2 \sim 1$. The moment of inertia $I$ of the $(N-1)$-particle system in $\Omega$-space, treated as a rigid body, is therefore approximately just $m^*$. For large $N$, the density of particles will be approximately uniform: the moment of inertia for such a uniform disk is just $\frac{1}{2}(N-1)m^*R^2 \sim \frac{1}{2}Nm^*R^2$, where $R$ represents the disk radius and $(N-1)m^*$ is the total mass. Hence $R^2 \sim \frac{2}{N}$, the average density of particles is $\frac{(N-1)}{\pi R^2} \sim \frac{N^2}{2\pi}$, and the average particle-particle spacing is $\sim \frac{2\pi}{N}$. Now consider the sum over energies $e_j^{(J)}$ from Eq. (51):

$$\sum e_j^{(J)} \sim \sum \frac{\hbar^2 \pi^2 [N_m]^2}{2m^* \alpha_j^2 \pi [4\pi]^2}.$$  

(54)

The quantity $\alpha_{j0}$ for particle $j$ in ring $m$ is approximately $m$ times the average particle-particle separation: i.e. $\alpha_{j0} \sim m \frac{2\pi}{N}$. Replacing the sum over $j$ by a sum over the rings $m$, and using the approximate result that there are $6m$ particles in ring $m$, yields

$$\sum_j e_j^{(J)} \sim \sum_m \frac{h^2 \pi^2 [N_m]^2}{64m^* \pi m^2} \sim \frac{27h^2 N^2}{8m^* \pi} \sum_1^{m_{max}} m,$$

(55)

where $m_{max}$ is the maximum ring number. $m_{max}$ is given approximately by the disk radius $R$ divided by the particle-particle separation. Hence $m_{max}^2 \sim \frac{N}{\pi}$. For large $m_{max}$, $\sum_1^{m_{max}} m \sim \frac{1}{2} m_{max}^2$. Hence

$$\sum e_j^{(J)} \sim \frac{27h^2 N^2}{16m^* \pi^2}.$$  

(56)

We require the average $e_j^{(J)}$ value, $\bar{e}$, with the average taken over all $j$. There are $N-2$ such $j$ coordinates, hence for large $N$ we have $\bar{e} \sim \frac{27h^2 N^2}{16m^* \pi}$ as claimed in Sec. IV. Given that

$$\tilde{\Delta} \sim 2 \frac{\delta a}{a} \bar{e},$$  

(57)

we obtain

$$\tilde{\Delta} \sim \frac{\delta a \cdot 27h^2 N^2}{8m^* \pi^2}.$$  

(58)
and hence $\tilde{\Delta} \sim N^2$ as claimed.

Second, we investigate the general $N$-dependence of $E_0$. Following Eqs. (47) and (48), we assume that $E_0$ is dominated by the classical potential energy at the SEM $\Omega' \equiv \Omega_0'$, i.e. $E_0 \sim \beta V(\Omega_0')$. This is consistent with our assumption throughout the paper of considering configurations close to the classical minima. Hence

$$E_0 \sim \beta \sum_{j<j'} \frac{1}{|\alpha_j \alpha_{j'} e^{i\theta_j} - \alpha_{j'} \alpha_j e^{i\theta_{j'}}|^2} .$$

(59)

Replacing the denominator by $\alpha^2$ yields $E_0 \sim \frac{\beta}{\alpha^2} \sum_{j<j'} 1$ and hence $E_0 \sim \beta N \frac{1}{2} (N-1)(N-2)$. For large $N$, $E_0 \sim \beta N^3$ and hence $E_0 \sim N^3$ as claimed. We note that while this derivation is crude, the final expression for $E_0$ is not actually used in the calculation of energy gaps. The only result used is the conclusion that $E_0 \gg \tilde{\Delta}$ for large $N$. 

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Figure Captions

Figure 1: Jacobi coordinates for the $N = 3$ electron system. Reading clockwise, the classical configuration for three repulsive particles $\Omega'_0 \equiv (132)$ corresponds to $(\alpha, \theta) = (\frac{\pi}{4}, \frac{\pi}{2})$ (i.e. $(x, y) = (0, 0)$); the other classical configuration $\Omega'_1 \equiv (123)$ corresponds to $(\alpha, \theta) = (\frac{\pi}{4}, -\frac{\pi}{2})$ (i.e. $(x, y) = (0, \pi)$ or, equivalently, $(0, -\pi)$).

Figure 2: Schematic diagram showing a portion of the hyperangular $\Omega'$-space. Two symmetrically equivalent minima (SEMs – labelled as $\Omega'_i$) are indicated by larger circles, while nearby symmetrically inequivalent minima (SIMs – labelled as $\Omega'_{i(a)}$) are indicated by smaller circles.

Figure 3: Contour plot of ficticious potential $V(x, y; \epsilon)$ in the $(x, y)$ plane for the $N = 3$ electron problem. The two symmetrically equivalent minima (SEMs – $\Omega'_0$ and $\Omega'_1$ from Fig. 1) are shown. Minima in $V(x, y; \epsilon)$ occur at $(0, 0)$ and $(0, \pm \pi)$ (i.e. at the classical configurations). Maxima occur at $(\ln \sqrt{3}, \pm \frac{\pi}{2})$, where $V(x, y; \epsilon) \to \infty$ (i.e. electrons 2 and 3 or 1 and 3 coincident). $V(x, y; \epsilon)$ is positive and finite everywhere else. The same qualitative features appear for all $\epsilon$ ($\frac{m^*}{m^*_B} = 5$ is used as an illustration).

Figure 4: Ground-state classical configuration for 230 electrons (black dots) calculated numerically using a Monte Carlo simulation. Figure adapted from Fig. 2 of Bedanov and Peeters (Ref. 14). Straight lines are drawn to bisect the midpoint between nearest neighbor electrons, thereby highlighting the approximately hexagonal local symmetry. Circles are drawn to illustrate the approximately ring-like arrangement of electrons. The inner circles only pass through regular hexagons. The outer circle passes through several pentagons and distorted hexagons because of its proximity to the edge of the finite cluster.

Figure 5: A particular symmetrically equivalent minimum (SEM – labelled in the text as $\Omega'_0$) with $N$ near the center (c.f. Fig. 4). We are considering the limit of large $N$. Ring $m$ is such that $N >> j >> 1$ and it is therefore far away from the circumference of the cluster.
Figure 6: Typical ring $m$ for the various spin-polarizations. Although only 12 particles are shown for clarity, the ring is assumed to contain a large number, i.e. $N_m \gg 1$ since $m \gg 1$.

(a) $N_+ : N_- = 1 : 1$. (b) $N_+ : N_- = 2 : 1$. (c) $N_+ : N_- = 3 : 1$.

Figure 7: Theoretical lower estimate (straight line) for FQHE energy gaps obtained from the present theory as compared to experimental results over a range of lower mobility GaAs heterostructure samples. (Figure adapted from the data of Boebinger et al., Refs. 27 and 3). Experimental data: $\nu = \frac{1}{3}$ (black points), $\nu = \frac{2}{3}$ (white points). As discussed in the text, theoretical gaps are same for $\nu = \frac{1}{3}$ and $\frac{2}{3}$ to a first approximation.

Figure 8: Theoretical upper (dashed line) and lower (solid line – same as Fig. 7) estimates for FQHE energy gaps obtained from the present theory as compared to experimental results over a range of higher mobility GaAs heterostructure samples. Data taken from Ref. 28 of Mallett et al. (squares) and Ref. 30 of Willett et al. (solid circles with error bars). Experimental data contains values for fractions $\nu = \frac{p}{3}$ where $p = 1, 2, 4, 5$. As discussed in the text, theoretical gaps are independent of $p$ to a first approximation.
