Electronic spectra and chemical potential of 2-D multi-electron quantum dots in magnetic field: exact multi-pole expansion of coulomb correlation

Priyanka Aggarwal1, Shivalika Sharma1, Harsimran Kaur, Sambhav Yadav and Ram Kuntal Hazra

Department of Chemistry (Physical), University of Delhi, Delhi 110007, India

E-mail: perkhias@gmail.com and rkhazra@chemistry.du.ac.in

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Abstract

Two-dimensional superlattices, TMDCs and graphene family exhibit strong coulomb correlations among e−e, e−h, electron-phonon and etc. As the number of electron \( N \) increases, confining gate voltage and transverse magnetic field are superseded by increasing coulomb interactions \( (N(N-1)/2 \) factors) that composes non-trivial Schrödinger equations. Representing such equations in Whittaker-M functions yields a modest alternate formalism, that accommodates integrals of coulomb (exchange) correlations in single-summed, finite and exact Lauricella functions via Chu-Vandermonde identity.

For higher carrier density \( (N = 3, 4, 5, 6, \ldots) \), the multipole expansion is incurred as exact and finite-summed coulomb, coulomb-type and dipole-type integrals. Although, fermionic exchange symmetry of many electron systems could be included in terms of various two-electron integrals, for the sake of brevity we have aimed to reproduce experimental results without spin. Signature of interplay among gate voltage, magnetic field, dielectric constant, mass and density of carriers is examined in electronic spectra, magnetization, chemical potential for the systems spanning over wide range of materials (He, BN, GaAs and etc.). Interestingly, chemical potential and addition energy as a function of magnetic field and number of carriers monitor the statistics between strongly degenerate to weakly degenerate composite fermions, coulomb blockade and shell structure of 2-D superlattices. At the most, quadrapole and octapole suffice the convergence.

1. Introduction

Confined ballistic systems such as quantum dots (0-D), quantum wires (1-D) and quantum wells (2-D) are engineered to study structural, optical, transport and magnetic properties of \( N \)-e systems by monitoring gate voltage, transverse magnetic field, dielectric constant and mass of carriers [1−4]. In addition to certain limitations on the issues like inclusion of Pauli exclusion principle, fermionic exchange symmetry, arbitrary magnetic and electric fields, as the number of correlation terms increases by a factor \( N(N−1)/2 \) an impenetrable barricade emerges in studying of such quantum systems. For 2-D quantum dots, Laughlin and Jain have set landmarks by introducing Laughlin’s wavefunction (LW) for 3−e and composite-fermion (CF) wavefunction for \( N \)-e systems respectively [5−7]. Other magnificent contributions in solving 2-D multi-electron systems have been improvised by Chakraborty et al, Hamaguchi et al and Taut [8−16]. Recently, our group proposed a modest alternate to many-body approximation methods for strong e−e and e−h correlations of 2-D quantum dots in magnetic field [17−19]. As many-body physics holds great importance, we have designed a prototype to solve exactly generalized \( N \)-e systems using multi-pole expansion (section 2) [20]. In this paper, synergistic coulomb- and dipole-type integrals evaluated by us are attributed to finitely single-summed terminated Lauricella function via Chu-Vandermonde identity [21]. In section 3, we have studied electronic spectra of 2−e, 3−e, 4−e and 5−e systems with respective chemical potential (\( \mu_N \)) and addition energy (\( \Delta \mu \)) to
explain extent of fermionic character, shell structure and coulomb blockade in detail. Chemical potential and addition energy as a function of gate voltage, magnetic field and number of electrons may reveal underlying physics related to phase transition and existence of both strongly and weakly degenerate character of unusually stabilized composite fermions [222]. In a dot structure, electrons are bound by a confining potential which gives rise to discretized energy states or shell structure of quantum dots with magic number $N = 2, 6, 12, 20$ representing the stable configurations [4].

2. Theoretical development

The spin free hamiltonian of 2-D $N$–e harmonically confined system ($\omega_0$) in transverse magnetic field having a vector potential ($A(r_i)$) of the form $A_i = \frac{1}{2}(B \times \nabla_i) = B(-y_i, x_i, 0)$ (symmetric gauge) can be cast as (in a.u.):

$$H = \sum_{i=1}^{N} \left\{ \frac{1}{2m_i} \left( \frac{p_i}{c} + \frac{1}{c} A(r_i) \right)^2 + \frac{1}{2} m_i \omega_0^2 r_i^2 \right\} + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{r_{ij}}$$

where $m_i$ and $c$ are effective mass of electron and static dielectric constant of the material respectively. Here, $H_i^0$ represents the unperturbed hamiltonian of the $i$th particle and $H'$ represent coulomb interaction term among charge carriers. For $N = 2$, the hamiltonion can be segregated into relative and center-of-mass coordinates [17]. But for $N > 2$, the interaction term ($H'$) replicates by a factor of $N(N-1)/2$. Moreover, surface integrals of both Dirichlet and Newman forms of Coulomb interaction in Green’s function expansion exhibit sharp falls in the values for harmonic oscillator and reach multiple expansion of generic coordinates ($r_i$). Thus, each interaction term ($H'$) is expanded via well known multi-pole expansion corroborating to [20]:

$$V = \frac{1}{\epsilon} \sum_{P=0}^{\infty} V_{P}^{(P)}$$

$V$ constitute all the interaction terms of $N$ electron into monopole ($P = 0$), dipole ($P = 1$), quadrupole ($P = 2$) and poles of higher order where

$$V_{m}^{(P=0)} = \frac{N - 1}{2} \sum_{i=1}^{N} \frac{1}{r_i}$$

$$V_{d}^{(P=1)} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{r_{ij}}{r_i^3}$$

$$V_{q}^{(P=2)} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left\{ \frac{3(r_{ij})^2}{r_i^4} - \frac{r_{ij}^2}{r_i^4} \right\}$$

Although, Schrödinger equations for both generic coordinates and relative/center-of-mass coordinates resemble to each other but their scaling factors differ [17]. Thus, it is very necessary to examine the non-relativistic equation for generic coordinates. Evaluating, $H_i^0 \xi_{n,m}^0 (r_i, \phi_i) = E_{n,m}^0 \xi_{n,m}^0 (r_i, \phi_i)$ for each $i$th particle of 2-D systems in magnetic field ($\omega_c = eB/\epsilon$) where, $n$ and $m$ are the principal and magnetic quantum numbers respectively.

$$\left\{ -\frac{1}{2} \left[ r_i^{-\frac{1}{2}} \frac{d^2}{dr_i^2} r_i^{\frac{1}{2}} + \frac{1}{r_i} \frac{\partial}{\partial r_i} \left( \frac{\partial}{\partial r_i} + \frac{1}{4} \right) \right] + i \omega_c \frac{\partial}{\partial \phi_i} \right\} \xi_{n,m}^0 (r_i, \phi_i) = m_i E_{n,m}^0 \xi_{n,m}^0 (r_i, \phi_i)$$

with $\xi_{n,m}^0 (r_i, \phi_i) = \frac{\omega_{0,n,m} u(r_i)}{\sqrt{2\pi} \sqrt{n!}}$, $m = 0, \pm 1, \pm 2, \ldots$ where $u(r_i)$ is a radial part of Schrödinger’s equation. Now, for every $i$th coordinate $H_i^0 \xi_{n,m}^0 = E_{n,m}^0 \xi_{n,m}^0$ results in
\[
\left\{ \frac{d^2}{dr^2} + \left( \frac{1}{4} - m^2 \right) \frac{1}{r^2} - m\omega_r - \Omega^2 r^2 + 2m_r E^0_{n,m} \right\}u(r) = 0
\]  
(8)

Converting \( u(r) \) \( \implies U(z) \) with \( z = \Omega r^2 \) and \( \Omega = \sqrt{m_r^2 \omega_r^2 + \frac{\gamma^2}{4}} \), equation (8) becomes:

\[
\left[ 4z \frac{d^2}{dz^2} + 2 \frac{d}{dz} + \left( \frac{1}{4} - m^2 \right) \frac{1}{z} - \frac{m\omega_r}{4z} - z + \frac{2m_r E^0_{n,m}}{4z} \right]U(z) = 0
\]  
(9)

Transformation of \( U(z) = z^{-1/2}M(z) \) leads to

\[
M''(z) + \left\{ \frac{1}{4} - \frac{m^2}{z^2} \right\} = \frac{1}{4} + \frac{\chi}{z} M(z) = 0
\]  
(10)

where \( \chi = (2m_r E^0_{n,m} - m\omega_r) / 4\Omega \) and \( M(z) \) is Whittaker-M functions. The \( i \)-th energy eigenvalue and normalized eigen function of \( N \)-particle systems is obtained as:

\[
m_r E^0_{n,m} = (2n + |m| + 1)\Omega + \frac{1}{2}m\omega_r \text{ and } \xi^0_{n,m}(z, \phi)
\]

\[
N_{n,|m|}z^{-\alpha(z)}M_{n,\nu}(z) = N_{n,|m|}z^{-\alpha(z)}M_{n,\nu}(z)
\]

\[
\text{where } N_{n,|m|} = \frac{\left( \Omega |m| + \frac{1}{2}m|m| \right)^{\alpha(z)}}{\alpha(z) \Gamma(\alpha(z))}, \text{ normalization constant}, \bar{\gamma} = \nu + n + \frac{1}{2} \text{ and } 2\nu = |m| \text{ (quantization condition)}.
\]

As far as the methodology deals with generic coordinates of all individual particles, Pauli exclusion principle (anti-symmetrization property) would nicely be achieved by straightforward formation of Slater determinants for open shell and closed shell configurations. In the succeeding sections we have deduced the \( e-e \) interaction in terms of monopole, dipole and quadrupole factors using variational approach.

2.1. Monopole factor

The integral of \( i \)-th monopole factor of \( e-e \) interaction (equation (4)) can be expressed as

\[
I_{n,m} = \int \xi(Z, \Phi) \frac{1}{\sqrt{\Omega}} \xi(Z, \Phi) \, dz
\]

where \( \xi(Z, \Phi) = \prod_{\alpha=1}^{12} \xi^0_{\gamma_i}(z_i, \phi_i) \).

The aforesaid factor finally be cast as:

\[
I = \frac{N_{n,|m|}N_{n,|m|}}{2\sqrt{\Omega}} \int_a^b \left( a_1, a_2 \right) M_{\bar{\gamma}, \nu} \left( z^{-\frac{1}{2}} a_1 \right) M_{\bar{\gamma}, \nu} \left( z^{-\frac{1}{2}} a_2 \right) \, dz
\]

(11)

where quantum numbers of all \( j = i \) coordinates and \( \nu \) are conserved (equation (4)). The integral is then evaluated as diagonal and off-diagonal component using the standard integral (equation (12)) [23, 24].

\[
\int_a^b x^{(\nu-1)} e^{-bx} M_{\bar{\gamma}, \nu} \left( a_1 x \right) M_{\bar{\gamma}, \nu} \left( a_2 x \right) \, dx = \frac{a_1 a_2 (b + A)^{-\nu} \Gamma(\nu + M)}{b + A}
\]

(12)

which satisfies the conditions \( Re(b + M) > 0 \) and \( Re\left( b \pm \frac{1}{2} \right) > 0 \). In equation (11), \( b = 0 \), \( a_1 = a_2 = 1 \), \( A = \frac{1}{2}(a_1 + a_2) = 1 \), \( \gamma = \frac{1}{2} \). The integral is then evaluated as diagonal and off-diagonal component using the standard integral (equation (12)).

\[
I = \frac{\left( \Omega |m| + |m|! \right)^{\nu} \left( m_1 + |m|! \right)^{\nu}}{\frac{m_1!(|m|)!^2}{m_1!(|m|)!^2}} \Gamma\left( \frac{|m| + 1}{2} \right)
\]

(13)

The Appell’s function \( F_2 \) is defined in terms of \( \text{F}_{1}\left( \frac{a, b, c}{d} \right) \) as [26]:

\[
F_2\left( \frac{|m| + 1/2, -n_1, -n_2; 1, 1}{|m| + 1, |m| + 1} \right) = \sum_{k=0}^{\infty} \left( \frac{|m| + \frac{1}{2}}{|m| + 1} \right)^k \frac{(-n_1)_k}{(n_2)_k} \times \frac{\Gamma\left( \frac{|m| + 1/2 + k}{|m| + 1} \right)}{\Gamma\left( \frac{1}{2} \right)}
\]

(14)

Now, summing \( F_2 \) by Chu-Vandermonde identity with the condition \( |m| + 1 > 0 \) we have [21],

\[
\text{F}_{1}\left( \frac{1}{|m| + 1} \right) = \left( \frac{-k + \frac{1}{2}}{|m| + 1} \right)^{n_2}
\]

(15)
Then, exploiting (equations (14), (15)) off-diagonal term (equation (13)) turned into single summed form as:

\[
I = \left\{ \frac{(\eta_1 + |m|)! \, (\eta_2 + |m|)!}{n! (|m|)!^2} \right\} \Gamma \left( |m| + \frac{1}{2} \right) \times \sum_{k=0}^{n} \left( \frac{|m| + \frac{1}{2}}{|m| + 1} \right) \langle -n \rangle_{k} \left( -k + \frac{1}{2} \right)_{n} \left( \frac{|m| + 1}{|m| + 1} \right)_{n} k! \right\}
\]

Similar employment of above methodology, the diagonal term appears as:

\[
I = \Omega^{2} \frac{(n + |m|)!}{n! (|m|)!^2} \Gamma \left( |m| + \frac{1}{2} \right) \sum_{k=0}^{n} \left( \frac{|m| + \frac{1}{2}}{|m| + 1} \right) \langle -n \rangle_{k} \left( -k + \frac{1}{2} \right)_{n} \left( \frac{|m| + 1}{|m| + 1} \right)_{n} k! \right\}
\]

where for any number ‘n’, Pochhammer symbol (\(n\)) = 1. The monopole contribution of other coordinates can similarly be extended to \(N\) electrons using (equation (4)). Alternatively, the same outcome (equations (16), (17)) can be achieved using \(s_{n,m}(x, \theta, \phi) = \frac{N'_{n,m} e^{- \frac{1}{2} z^2} L_{n}^{m}(z) \frac{\epsilon_{\text{ion}}}{\epsilon_{\text{ion}}'}}{\sqrt{\pi} \Gamma (n + 1)}\) where \(N' = \frac{25 \Gamma (n)}{\Gamma (n + 1) |m|!} \), \(L_{n}^{m}(z)\) is an associated Laguerre polynomials and standard integral of the forms [23, 27]:

\[
\int_{0}^{\infty} x^{(\sigma - 1)} e^{-\beta x} L_{n}^{m}(\alpha_{1} x) L_{m}^{n}(\alpha_{2} x) dx = (-1)^{\alpha_{1} + \alpha_{2}} \left( -\alpha_{1} - 1 \right) \left( -\alpha_{2} - 1 \right) b^{-\sigma} \Gamma (\sigma) \times F_{2} (\sigma; -n_{1}, -n_{2}; a_{1} + 1, a_{2} + 1; \frac{\alpha_{1}}{\alpha_{2}}, \frac{\alpha_{2}}{\alpha_{1}})
\]

where \(Re(\sigma) > 0, Re (b) > 0, \)

\[
\int_{0}^{\infty} e^{-x} x^{(\sigma + \frac{\alpha + \beta}{2})} L_{n}^{m}(\alpha_{1} x) L_{m}^{n}(\alpha_{2} x) dx = (-1)^{k} \frac{\Gamma (1 + \mu + k)}{kl_{\alpha}^{\mu+\beta}} \times \sum_{t=0}^{k} \frac{\alpha_{2}^{t}}{\alpha_{1}^{t}} \Gamma (1 + \beta + t) \Gamma (1 + \mu + t) \times \frac{P_{t}^{\mu,\beta}(z)}{t!} \frac{(-a_{0} + \alpha_{1} + \alpha_{2})}{2}
\]

\[
\left[ Re \left( s + \frac{\alpha_{1} + \alpha_{2}}{2} \right) > 0, a_{1} > 0, a_{2} > 0, Re (\mu + \beta) > -1 \right]
\]

2.2. Dipole factor

Individual integral of first order dipole factor (equation (5)) can be expressed as:

\[
I_d = \frac{1}{2} \left\{ \Xi (Z, \Phi) \right\} \left| \frac{\mathbf{j}_{r_{1}} \cdot \mathbf{r}_{2}}{|r_{1}|^3} \right| \Xi (Z, \Phi)
\]

In order to decouple the operator, the discretized projection over a complete basis set of the form \(\sum_{l=0}^{L} \Xi (Z, \Phi) / \ni (Z, \Phi) / \Xi (Z, \Phi)\) is inserted leading to [28]:

\[
I_d = \frac{1}{2} \sum_{l=0}^{L} \Xi (Z, \Phi) \left| \frac{\mathbf{j}_{r_{1}} \cos (\phi_{l})}{r_{1}} \right| \Xi (Z, \Phi) \times \left( \Xi (Z, \Phi) \right) \left| \frac{1}{r_{1}} \right| \Xi (Z, \Phi)
\]

Unwinding \(I_d\) into individual \(i^{th}, j^{th}\) and \(k^{th}\) space as:

\[
I_d = \frac{1}{2} \sum_{l=0}^{L} I_{d_{i}} I_{d_{j}} I_{d_{k}} \times I_{d_{i}}
\]

where,

\[
I_{d_{i}} = \left< \mathbf{n}_{i,j}, \mathbf{z}_{l} \right| M_{r_{1}, l}, \mathbf{r}_{l} \left| \mathbf{n}_{i,j}, \mathbf{z}_{l} \right> M_{r_{1}, l}, \mathbf{r}_{l}\right>,
\]

\[
I_{d_{j}} = \left< \mathbf{n}_{i,j}, \mathbf{z}_{l} \right| M_{r_{1}, l}, \mathbf{r}_{l} \left| \mathbf{n}_{i,j}, \mathbf{z}_{l} \right> M_{r_{1}, l}, \mathbf{r}_{l}\right>,
\]

\[
I_{d_{k}} = \left< \mathbf{n}_{i,j}, \mathbf{z}_{l} \right| M_{r_{1}, l}, \mathbf{r}_{l} \left| \mathbf{n}_{i,j}, \mathbf{z}_{l} \right> M_{r_{1}, l}, \mathbf{r}_{l}\right>
\]
Here, equation (22) is composed of coulomb-type \((I_{d_q}, I_{d_k})\), dipole-type \((I_{d_1})\) and angular momentum type integrals \((I_{d_3})\). Coulomb-type integral \((I_{d_q}, I_{d_k})\) is treated in a similar fashion alike monopole factor (section 2.1). The dipole-type integral \((I_{d_1}(m_1, |m_2|, n_2, |m_2|))\) for every \(z_j\) coordinates can be represented as:

\[
I_{d_1} = \frac{N_{m_2} |m_2|}{2\Omega^2} (z^\pm M_{n_2, |m_2|}(z) M_{n_2, |m_2|}(z))
\]

Using the Chu-Vandermonde identity [21] and the standard integral (equation (12)) satisfying the conditions \(Re (\varphi + \kappa) > 0\) and \(Re (b + \frac{1}{2}a_1 + \frac{1}{2}a_2) > 0\) where \(b = 0, a_1 = a_2 = 1, A = \frac{1}{2}(a_1 + a_2) = 1, \gamma_1 = \pm \nu_1 = \pm \nu_2 = \frac{1}{2}, M = \gamma_1 + \gamma_2 = \frac{1}{2} + 1, \varphi = \frac{1}{2}, \gamma_2 = 0, 1, 2, \ldots; \kappa - \gamma - 1/2 = 1, 2, \ldots\), the integral manifests in single summation as:

\[
I_{d_1} = \left[ \frac{1}{\Omega} \frac{(m_1 + |m_2|)! (n_2 + |m_2|)!}{n_2!(|m_2|)!^2} \sum_{k=0}^{\min(n_2, |m_2|)} \left(\frac{|m_2| + |m_2| + 2}{2}\right)\right]
\]

Now, evaluating angular momentum \((I_{d_3})\):

\[
I_{d_3} = \frac{1}{2} \delta_{m_1,0} |m_2, \pm 1, m_2, \pm 1| + \delta_{m_1,0} |m_2, 1, m_2, 1| + \delta_{m_1,0} |m_2, 1, m_2, 1| + \delta_{m_1,0} |m_2, 1, m_2, 1|
\]

Substituting (equations 24), (25) and coulomb-type integrals \((I_{d_q}, I_{d_k})\) section 2.1 in (equation 22) to obtain dipole factor which can be extended to \(N\) electrons using equation (5).

2.3. Quadrupole factor

The integral representation of second order quadrupole contribution (order of pole \(\mathcal{P} = 2\)) (equation (6)) reads as:

\[
I_q = \left\langle \Xi(Z, \Phi) \right| \frac{3\gamma_j - \text{r}_j^2}{|\vec{r}_j|^3} - \frac{\gamma_j^2}{|\vec{r}_j|^5} \left\rangle \Xi(Z, \Phi)
\]

Simplifying the integral we get:

\[
I_q = \left\langle \Xi(Z, \Phi) \right| \frac{3\gamma_j^2 \cos^2(\phi_j)}{|\vec{r}_j|^3} - \frac{\gamma_j^2}{|\vec{r}_j|^5} \left\rangle \Xi(Z, \Phi)
\]

It further reduces to:

\[
I_q = \left\langle \Xi(Z, \Phi) \right| \frac{\gamma_j^2}{|\vec{r}_j|^3} (3 \cos^2(\phi_j) - 1) \left\rangle \Xi(Z, \Phi)
\]

The operator is decoupled again by inserting discretized projection of the form \(\sum_{l=0}^{\infty} \Xi_l(Z, \Phi) \langle \Xi_l(Z, \Phi) \rangle\) [28]. Factorizing \(I_q\) in individual \(l\)th, \(j\)th and \(h\)th coordinates (projection operator) leads to:

\[
I_q = \sum_{l=0}^{\infty} \Xi_l(Z, \Phi) \langle \Xi_l(Z, \Phi) \rangle\)

where,

\[
I_{q_1} = \left\langle N_{0, z_j} | z_j^{\pm 1} M_{m_1, |m_2|}(z) \right| N_{n_2, z_j} | z_j^{1/2} M_{m_2, |m_2|}(z) \rangle
\]

\[
I_{q_2} = \left\langle N_{0, z_j} | z_j^{\pm 1} M_{m_1, |m_2|}(z) \right| \frac{1}{\gamma_j} \left| N_{n_2, z_j} | z_j^{1/2} M_{m_2, |m_2|}(z) \rangle \right.
\]

\[
I_{q_3} = \left( \frac{\delta_{m_1,0} e^{m_1/2} e^{m_2/2} |3 \cos^2(\phi_j) - 1|}{\sqrt{2\pi}} \right)
\]

\[
I_{q_4} = \left( \xi_{0, z_j}^{m_1, m_1} \right| \frac{1}{\gamma_j} \left| \xi_{n_2, z_j}^{m_2, m_2} \right)
\]

Here, equation (29) consists of angular momentum type \((I_{q_1})\), coulomb-type \((I_{q_2}, I_{q_3})\) and square-position-type integrals \((I_{q_4})\). Coulomb-type integral is treated similar to monopole factor (section 2.1). Unwinding \(I_{q_4}\) and inserting discretized projection operator of the form \(\sum_{k=0}^{\infty} \Xi_k(Z, \Phi) \langle \Xi_k(Z, \Phi) \rangle\)
\[ I_{q_1} = \sum_{k=0}^{\infty} \left( \xi^0_{n_{k,i}l_{mi,f}j} \right) \frac{1}{r^2} \delta_{n_{k,i}l_{mi,f}j} \delta_{m_{k,i}l_{mi,f}j} \times \left( \xi^0_{n_{k,i}l_{mi,f}j} \right) \delta_{n_{k,i}l_{mi,f}j} \delta_{m_{k,i}l_{mi,f}j} \]  

(30)

The square-position-type integral \( I_{q_1} (n_a, |m_1|, n_b, |m_2|) \) for every \( z_i \) coordinates can be written as:

\[ I_{q_1} = \frac{N_{n_1}m_1|N_{n_2}m_2|}{2\Omega^2} (z^0_{M_{n_i},x_i}(z) M_{M_{n_i},x_i}(z)) \]  

(31)

Chu-Vandermonde identity [21] is exploited and the standard integral (equation (12)) which satisfies the conditions \( Re(b + M) > 0 \) and \( Re\left( b \pm \frac{1}{2}a_i \pm \frac{1}{2}a_j \right) > 0 \) where \( b = 0, a_i = a_j = 1, A = \frac{1}{2}(a_i + a_j) = 1, \) \( \gamma_i - \frac{1}{2} = \frac{m_i}{2}, \gamma_j - \frac{1}{2} = \frac{m_j}{2}, M = \gamma_i + \gamma_j = \frac{m_i}{2} + \frac{m_j}{2} + 1, \varphi = 1, 2, \gamma = 0, 1, 2, \ldots; k = \gamma - 1/2 = 0, 1, 2, \ldots \). The integral leads to single summation as:

\[ I_{q_1} = \frac{1}{\Omega} \left( \frac{(m_1 + |m_2|)! (m_2 + |m_1|)!}{n_1! (|m_1|)!^2} \delta_{n_1,0} \right) \frac{1}{2} \left( \frac{|m_1| + |m_2| + 4}{2} \right) \times \sum_{k=0}^{n_1} \left( \frac{|m_1| + |m_2| + 3}{2} \right) (-1)^k \left( \frac{|m_1| - |m_2| - 1}{2} \right) \frac{1}{2} \right) \]  

(32)

Now, calculating angular momentum \( I_{q_1} \):

\[ I_{q_1} = \frac{3}{4} \left( \delta_{m_1,0,m_2,2} \right) \times \delta_{m_1,0,m_2,2} + 2 \left( \delta_{m_1,0,m_2,2} \times \delta_{m_1,0,m_2,2} \right) - \delta_{m_1,0,m_2,2} \times \delta_{m_1,0,m_2,2} \]  

(33)

Substituting (equation (32), (33)) and coulomb-type integrals \( I_{q_1}, I_{q_2} \) (section 2.1) in (equation (29)) to obtain quadrupole contribution factor which can be extended to \( N \) electrons using (equation (6)).

3. Result and discussion

The onset of inter-electronic repulsions constitutes mixing among states of atoms, molecules, superlattices and quantum dots due to massive interplay of correlations in comparison to quadrapole factor. Contribution of monopole factor to Coulomb (exchange) integral can roughly be formulated as (quantum number of all other coordinates are conserved) [17]:

\[ \left( \xi_{0,m_i} \right) \frac{1}{r} \left( \xi_{0,m_i} \right) \simeq \frac{1}{\epsilon \sqrt{|m| + \frac{1}{2}}} \]  

(34)

for bound states, nearly equating to Laughlin’s prediction of \( 1/\sqrt{|m|} \) for states having higher angular moment \( m \) and high \( \omega_q \). A key point to be noted is that states of conserved angular momentum \( (m_1 = m_2 = m_3 = \ldots = m) \) mutually exclude dipole contribution. Our formalism of absolutely terminating coulomb- and dipole type integrals does not meet any secular divergence problem at all [11]. Level spacing statistics and specific heat measurements \( (C_v) \) are also investigated in detail. It is evident that switching over of statistics between Poisson and Wigner distribution is very much prominent for \( N = 2 \) in comparison to \( N = 3, 4, 5, 6 \ldots \) and consequently, \( C_v \) shows maximum fluctuations for \( N = 2 \) rather than the cases of higher carrier density [17]. Therefore, for the brevity and compactness of the paper we have refrained to discuss it.

3.1. Energy level diagram

The electronic structures of different materials \( [He, Li, Be, GaAs and BN] \) scrutinized with \( N = 2, 3, 4, 5 \) at \( \omega_q = 0.004 \) a.u. and \( 0.000 04 \) a.u. for different \( m_i \) and \( \epsilon \) \( (He, Li and Be) \) \( (m_i = 1.0 \) a.u. and \( \epsilon = 1.0) \), \( GaAs \) \( (m_i = 0.07 \) a.u. and \( \epsilon = 12.35) \) and \( BN \) \( (m_i = 0.26 \) a.u. and \( \epsilon = 7.1) \) register an unusual pattern on energy spectra (figures (1–2)). In our previous work we have discussed energy level diagram of \( SiO_2 \) \( (m_i = 0.42 \) a.u. and \( \epsilon = 3.9) \). But here, we have excluded \( SiO_2 \) \( (m_i = 0.42 \) a.u. and \( \epsilon = 3.9) \) system. Although, it also required a detailed discussion for \( SiO_2 \) with varying carrier density, size and confinements, for the sake of brevity we have refrained from the corresponding results [17]. An enhancement in energy levels with increasing carrier density \( (N = 2, 3, 4, 5) \) is noteworthy for atomic systems \( (He, Li, Be) \) in comparison to other systems \( (GaAs and BN) \).
because of low dielectric constant. In general, lowering of the confinement frequency by 10 times, a relative decrease in coulomb interaction nearly by three times is observed in comparison to non-interacting energy (equation (34)) [17]. In the next section we will discuss the role of confinement frequency ($\omega_0$) on energy spectrum.

3.1.1. Strong confinement systems ($\omega_0 = 0.004$ a.u.)

In strongly confined systems, apparently weak correlations marks a feeble blow on energy spectrum. But for systems with higher mass ($m_e$) and lower dielectric constant ($\varepsilon$), it appears little disordered. The early crossing of ground state shifts monotonically to lower field ($\omega_c = 0.0009$ a.u., 0.0004 a.u. and 0.0003 a.u.) with increasing carrier density (figures 1(g)–(i) GaAs system). In BN quantum dots (figures 1(d)–(f)), multiple transitions with stabilization of ground state is observed at weak field ($\omega_c = 0.0$ a.u. to 0.0015 a.u.) for $N = 3$ on account of interplay between enhanced exchange correlation and magnetic field (figure 1(e)). The stabilization becomes more pronounced for $N = 4$ (figure 1(d) BN system). Atom-like quantum dots (figures 1(a)–(c)) imitate exceptional features of crossings/anti-crossings, stabilizations and enhanced degeneracies in lower bound states as a function of $N$. For $N = 2$ (He), the nodeless ground state at $\omega_c = 0.0$ comprises of huge crossing/anti-crossing at moderate $\omega_c = 0.001$ a.u., 0.002 a.u., 0.004 a.u.) (figure 1(c)). However, an immense stabilization of lower bound states for $N = 3$ and doubly degenerate ground state with quick evolution is recognized for $N = 4$ (figures 1(a), (b)).

Figure 1. Energy level Diagram of 2-D of $N$-e quantum dot systems with $\omega_0 = 0.004$ a.u. as a function of magnetic field ($\omega_c$) for $N = 2$ (c, f) and (i), $N = 3$ (b, e and h) and $N = 4$ (a, d) and (g): (a)–(c) ($\varepsilon = 1.0$ and $m_e = 1.0$ a.u.), (d)–(f) ($\varepsilon = 7.1$ and $m_e = 0.26$ a.u. BN) and (g)–(i) ($\varepsilon = 12.35$ and $m_e = 0.07$ a.u. GaAs)) (redline : ground state and blue line : excited state).
3.1.2. Weakly confined systems \( (\omega_0 = 0.000\, 04 \text{ a.u.}) \)

Inter-electronic repulsions greatly suppress magnetic field at weaker confinement \( (\omega_0 = 0.000\, 04 \text{ a.u.}) \) depending upon the number of carriers and static dielectric constant. As a result of it, symmetry of lower bound states is destroyed and the ground state become more involved in crossings/anti-crossings as the survey spans over \( \epsilon = 1.0 \) (atomic) to \( \epsilon = 7.1 \) (BN) and \( \epsilon = 12.35 \) (GaAs). Exchange interactions cause massive stabilization, enhanced degeneracy of ground state and numerous transitions among lower bound states for \( N = 3 \) and \( N = 4 \) electrons (figures 2(b), (e), (h) (a), (d), (g)). Ground state remains doubly degenerate in case of atom-like quantum dots and criss-crossing among states is diminished due to acute upsurge of coulomb interactions for high carrier density (figure 2(a)). The similar impression of excess stabilization and/or enhanced degeneracy among lower bound states is recognized for either low dielectric systems with low carrier density \( (N=3, \epsilon=1.0) \) or high dielectric systems with high carrier density \( (N=4, \epsilon=7.1) \) (figures 2(g), (e) (b), (c), (d) and (1(d) 2(g)), (1(b) 2(e))). Particularly, in case of BN (Figures 2(d)–(f)) and GaAs (figures 2(g)–(i)) quantum dots, enhanced exchange interactions cause unusual stabilization and shuffling of few lowest bound states in weak field regime for \( N = 3 \) (figures 2(e), (h)). But as \( N \) increases doubly degeneracy of ground state or excess stabilization or both appears due to profound coulomb (exchange) interaction (figures 2(d), (g)).

3.2. Magnetization \( (M) \)

Magnetization is another aspect that highlights the proliferating effect of coulomb interaction with increasing \( N \) through sharp discontinuities as a function of magnetic field \([29, 30]\). It can be expressed as (within the low temperature limit \( T \sim 1\, \text{K} \)) [31].

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**Figure 2.** Energy level Diagrams of 2-D \( \text{N}-\epsilon \) quantum dot systems with confinement frequency \( (\omega_0) = 0.000\, 04 \text{ a.u.} \) as a function of magnetic field \( (\omega) \) for \( N=2 \) (c), (f) and (i), \( N=3 \) (b), (e) and (h) and \( N=4 \) (a), (d) and (g): (a)–(c) \( (\epsilon=1.0 \text{ and } m_e=1.0 \text{ a.u.}), \) (d)–(f) \( (\epsilon=7.1 \text{ and } m_e=0.26 \text{ a.u.} \text{ (BN)} ) \) and (g)–(i) \( (\epsilon=12.35 \text{ and } m_e=0.07 \text{ a.u.} \text{ (GaAs)} ) \) (redline: ground state and blue line: excited state).
Smooth decay in magnetization curves for low dielectric system or results in level crossings changing angular momentum of lowest bound states. Even at ground state transitions near crossing points (figures 3(c), (f)) these transitions primarily address change in angular momentum of ground state. Even at \( \omega_c = 0.0 \) a.u., a quantitative difference in magnetization is noticed. In GaAs system, coulomb interaction diminishes further and results in smooth curve for systems of dielectric constant for GaAs (\( m_e = 0.07 \) a.u. and \( \epsilon = 12.35 \)) with \( \omega_{c1} = 0.004 \) a.u. and \( \omega_{c2} = 0.000 \) a.u. investigated.

### 3.2.1. Weakly confined system (\( \omega_0 = 0.000 \) a.u.)
A sharp jump in magnetization for \( N = 4 \) and little step wise decrease for \( N = 2, 3 \) is observed in low dielectric system (\( \epsilon = 1.0 \)). In BN system, two sharp jumps in the curve (\( \mathcal{H} - \omega_c \)) at two different magnetic field (\( \omega_c \sim 0.008 \) a.u. and \( 0.001 \) a.u.) for \( N = 4 \) and single jump for \( N = 2 \) (\( \omega_c \sim 0.001 \) a.u.) are observed (figure 3(b)). It is seen that number of jumps (discontinuities) have reduced in comparison to weakly confined systems because of increasing confinement frequency scales down the strength of coulomb interaction. In GaAs system, coulomb interaction diminishes further and results in smooth curve for \( N = 2 \) (figure 3(c)).

### 3.2.2. Highly confined system (\( \omega_0 = 0.004 \) a.u.)

3.3. Chemical potential (\( \mu_N \)) and addition energy (\( \Delta \mu \))

Level crossings/anti-crossings in energy level diagram appear as cusp or transition in chemical potential with changing angular momentum of lowest bound states. The number of transitions or cusps is either enhanced or results in fluctuation with number of electrons, dielectric constant (\( \epsilon \)), mass of carrier (\( m_e \)), confinement frequency (\( \omega_0 \)) and magnetic field (\( \omega_c \)). Thus, in this section a variation of chemical potential...
and the addition energy (energy required to add a charge)

$$\left( \frac{\partial E}{\partial N} \right)_f$$

as a function of magnetic field ($\omega_c$) and number of electrons ($N$) with $\omega_0 = 0.004$ a.u. and $\omega_0 = 0.000 04$ a.u. at $T \sim 10$ K for GaAs, BN and atom-like quantum dot is examined.

3.3.1. Strongly confined regime ($\omega_0 = 0.004$ a.u.)

- Gallium Arsenide (GaAs) quantum dots ($\epsilon = 12.35$ and $m_e = 0.07$ a.u.): Magnetic-field dependence of $\mu_1$ is reflected in the smooth curve due to absence of crossings/anti-crossings of the ground state (figure 4(a)). But with the onset of coulomb interaction a very small cusp emerges at $\omega_c = 0.000 9$ a.u. in $\mu_2$ whereas $\mu_3$ and $\mu_4$ exhibit prominent cusps or transitions at $\omega_c = 0.000 45$ a.u. and $\omega_c = 0.000 320$ a.u. respectively in contrast to $\mu_1$ and $\mu_2$ (figure 4(a)). The transitions at $\omega_c = 0.000 2$ a.u., $0.000 3$ a.u. and $0.000 45$ a.u. are observed for $\mu_5$. These discontinuities in the form of maxima and minima in chemical potential may give an impression of fractional Landau level filling factors [32, 33]. The gap between $\mu_1$ and $\mu_2$ appears to be constant which indicates equal synergistic effect of coulomb interaction on lowest bound states for zero and non-zero magnetic field (figures 4(a)). Moreover, addition energies are also plotted against the number of electrons $N$ at different magnetic fields which map to the 'shell structure' already reported by Kouwenhoven and his group [4] at $B = 0$ for strongly confined system (figure 4(c)). The peak structure fades away gradually into a smooth curve at high magnetic field ($\omega_c = 0.001$ a.u.). High magnetic field compacts electrons and increases interactions to such an extent that shuffling among states is reduced. In case of GaAs, chemical potential and addition energy plots partially resemble to the non-interacting system due to reduced coulomb interaction.

Figure 4. Chemical potential ($\mu_N$) versus magnetic field ($\omega_c$) for $N = 1-5$ (figures (a), (b) ($\omega_0 = 0.004$ a.u., 0.000 04 a.u. respectively)) and Addition energies ($\Delta \mu$) versus number of electrons ($N$) in different magnetic field (figures (c), (d) ($\omega_0 = 0.004$ a.u., 0.000 04 a.u. respectively) of 2-D $N$-e GaAs quantum dot.
Boron Nitride (BN) quantum dots ($\epsilon = 7.1$ and $m_e = 0.26$ a.u.): A smooth curve of $\mu_1$ against magnetic field $B$ expectedly appears owing to absence of cross over points among lowest bound states (figure 5(a)). The appearance of cusp or transition of $\mu_2$ at $\omega_c = 0.0015$ a.u. becomes more prominent than that of GaAs quantum dot due to enhanced e-e interaction (figures 4(a)–5(a)). $\mu_3$ decreases up to a threshold magnetic field ($\omega_c = 0.0014$ a.u.) and then increases with increasing magnetic field (figure 5(a)). This peculiar behavior is ascribed to the enhanced exchange interactions in low field which may emerge as a remnant of switch over from strongly degenerate to weakly degenerate fermionic character. There are two cusps in $\mu_2$ at $\omega_c = 0.0006$ a.u. and at $\omega_c = 0.0024$ a.u. due to crossing of ground state for $N = 3$ and $N = 4$ dots (figure 5(a)). However, $\mu_5$ remains nearly constant up to certain magnetic field ($\omega_c = 0.008$ a.u.) and then a steep increase with increasing magnetic field on account of upsurging coulomb interaction due to enhanced carrier density. These oscillations, i.e., rise and fall in chemical potential reflect acute response of dots to magnetic field and number of particles ($N = 2, 3, 4, 5, \ldots$) (figure 5(c)). At low magnetic field ($= 0.0$ a.u. and $0.0008$ a.u.), an experimentally observed ‘shell structure’ is observed which inverts at high magnetic field ($= 0.0016$ a.u., $0.0024$ a.u., $0.0032$ a.u. and $0.004$ a.u.) due to augmentation of coulomb interaction (figure 5(c)).

Atom-like quantum dots ($\epsilon = 1.0$ and $m_e = 1.0$ a.u.): The characteristics of ground and few excited states are very distinctive in atom-like quantum dots ($\epsilon = 1.0$, $m_e = 1.0$ a.u.) than that of BN ($\epsilon = 7.0$, $m_e = 0.26$ a.u.) and GaAs ($\epsilon = 12.35$, $m_e = 0.07$ a.u.) systems. Therefore, chemical potential and addition energy respond differently. Absence of cusps in $\mu_2$ and $\mu_3$ signifies no level crossing/anticrossing of the ground states. Anomalously, $\mu_3$ has a huge fall and lies far below $\mu_2$, with the onset of magnetic field (figure 6(a)). This is due to enhanced exchange interactions which cause excess stabilization to the $N = 3$ system. $\mu_4$ and $\mu_5$ show similar trend but a little cusp near $\omega_c = 0.005$ a.u. is observed in $\mu_4$. Interestingly, the spacing between $\mu_2$ and $\mu_4$ is extremely small in comparison to $\mu_5$ and $\mu_4$ and $\mu_5$ which exhibit deviation from the behavior.
reported by Tarucha et al [34] for moderate and high dielectric quantum dots (figure 6(a)). Addition energy plot also displays a complete opposite trend in comparison to the usual shell structure (figure 6(c)). It is clearly evident from the studies of chemical potential and addition energy that formation of tightly bound composite-fermions is highly facilitated by magnetic field for \( N = 2 \) and 3 than that of \( N = 4 \) and 5 which is a reminiscence of Cooper pair formation.

3.3.2. Weakly confined system (\( \omega_0 = 0.000 04 \text{ a.u.} \))

Coulomb repulsion profoundly dominates in larger dots which brings about a noticeable effect in chemical potential and addition energies. Thus, study of larger dots displays different signature in chemical potential and addition energy plots.

- Gallium Arsenide (GaAs) system (\( \epsilon = 12.35 \) and \( m_e = 0.07 \text{ a.u.} \)): Similar impression of nearly smooth curve appears for \( \mu_1 \) and \( \mu_2 \) as there is negligible e–e coulomb correlation (figure 4(b)). Alike strongly confined atom-like quantum dots a monotonic decrease in \( \mu_3 \) is found due to unusual stabilization induced by exchange interactions. A sharp increase with magnetic field is observed for \( \mu_4 \) and \( \mu_5 \). The energy gap between \( \mu_3 \) and \( \mu_4 \) widens up with increase in magnetic field (figure 4(b)). Subsequently, addition energy follows opposite trend to that of highly confined GaAs system and the corresponding peaks become sharp with increase in magnetic field (figure 4(d)).

- Boron Nitride (BN) system (\( \epsilon = 7.1 \) and \( m_e = 0.26 \text{ a.u.} \)): \( \mu_1 \) shows an increasing behaviour whereas \( \mu_2 \) and \( \mu_3 \) decreases with the arrival of cyclotron frequency. \( \mu_2 \) and \( \mu_3 \) coincide with \( \mu_1 \) near \( \omega_c = 0.000 025 \text{ a.u.} \) (figure 5(b)). However, \( \mu_4 \) and \( \mu_5 \) increases as usual with magnetic field (figure 5(b)). The widening of energy gap between \( \mu_2 \) or \( \mu_3 \) and \( \mu_4 \) is also noticeable in BN system. Addition energy plot against number of electrons

Figure 6. Chemical potential (\( \mu_N \)) versus magnetic field (\( \omega_c \)) for \( N = 1-5 \) (figures (a), (b) (\( \omega_0 = 0.004 \text{ a.u., 0.000 04 a.u. respectively} \)) and Addition energies (\( \Delta \mu_N \)) versus number of electrons (\( N \)) in different magnetic field (figures (c), (d) (\( \omega_0 = 0.004 \text{ a.u., 0.000 04 a.u. respectively} \)) of 2-D \( N \)-e atom-like quantum dot.
are also similar to that of highly confined atom-like quantum dots at low and intermediate magnetic field (figure 5(d)). In case of high magnetic field ($\omega_c = 0.000 \ 032 \ \text{a.u.}$ and $0.000 \ 04 \ \text{a.u.}$), addition energy increases for $N = 2$ which is a reversed trend to that of highly confined atom-like quantum dots (figure 5(d)).

- Atom-like quantum dots ($\epsilon = 1.0$ and $m_e = 1.0 \ \text{a.u.}$): Almost identical trends for chemical potential vs magnetic field ($\omega_\text{c}$) and addition energies against number of electrons ($N$) have been ascertained (figures 6(b), (d)). The only difference is with the magnitude of chemical potential and addition energies at different magnetic fields. It depicts reduction of competing behavior between coulomb interaction and confinement frequency that results in no significant change in chemical potential and addition energies (figures 6(b), (d)).

4. Conclusion

Hamiltonian of 2-D $N-e$ ($N = 2, 3, 4, 5, ...$) is a long-standing problem of non-relativistic quantum systems. The $N-e$ Schrödinger equation is expanded using multipole expansion into monopole, dipole, quadrupole and poles of higher orders by inserting discretized projection operator of a complete basis set over confluent hypergeometric Whittaker-M functions. It can bypass all secular divergence problems. Despite, the poles of all orders compliance with power law of length-scale in both negative and positive integers, integrals of multipole expansion invariably terminate at single summed hypergeometric series via Chu-Vandermonde identity and the orders compliance with power law of length-scale in both negative and positive integers, integrals of multipole expansion invariably terminate at single summed hypergeometric series via Chu-Vandermonde identity and the orders compliance with power law of length-scale in both negative and positive integers, integrals of multipole expansion invariably terminate at single summed hypergeometric series via Chu-Vandermonde identity and the orders compliance with power law of length-scale in both negative and positive integers. Exploiting such formalism to study quantum dots (GaAs, BN and atom-like) reveals intricate, detail and unusual behaviour of wide variety of systems. Multiple transitions or immense stabilization among lowest bound states occur with increasing carrier density. The enhanced degeneracies and stabilization emerge as a result of augmented exchange interactions among carriers. The appearance of smooth curves in magnetization for $N = 2, 3$ and 4 of weakly confined atom-like dot signify the effect of enhanced coulomb interactions. However, Sharp discontinuities or step order decrease in magnetization may give signature of phase transitions. The finer feature of decrease in chemical potential with magnetic field represents the existence of composite fermions, an indication of Cooper-pair formation. Moreover, shell structure of quantum dots maps only with weakly interacting fermi gases but brings about complete opposite trend in strongly interacting fermions.

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ORCID iDs

Ram Kuntal Hazra @ https://orcid.org/0000-0003-0787-431X

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