Charge and spin density waves: Quasi one dimension to two dimensions

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Abstract

Electronic charge and spin separation leading to charge density wave and spin density wave is well established in one dimensional systems in the presence and absence of Coulomb interaction. We start from quasi one dimension and show the possibility of such a transition in quasi one dimension as well as in two dimensions by going to a regime where it can be shown for free electrons that just interact via Fermi statistics. Since Coulomb interaction can only facilitate the phenomenon, the purpose of our work is to show the phenomena unambiguously in the limit when Coulomb interaction can be ignored. Finally we also comment on dimensions greater than two and including Coulomb interactions.

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I. INTRODUCTION

Linear superposition principle in quantum mechanics tells us that spontaneous symmetry breaking is not possible in quantum mechanics as the infinite number of degenerate states that are associated with spontaneous symmetry breaking can superpose to give a general state that has the same symmetry as the Hamiltonian. In spite of it, certain heavy nuclei exhibit rotational excitations, that can not be explained by the shell structure alone of a spherical nucleus. Initial understanding of this was provided by Bohr and Mottelson\textsuperscript{1} in terms of collective modes of oscillation of a deformed nucleus. Such nuclear deformation may well be due to spontaneous symmetry breaking. However as nuclear forces and nuclear Hamiltonian are still not precisely known, a first principle quantum mechanical analytic understanding is not yet possible. Similar ideas of spontaneous symmetry breaking can also explain the details of the mass spectra of alkali metal clusters and indicate the existence of a spin-density wave in quantum dots\textsuperscript{2–5}.

In these systems, since earlier days, researchers have approached the problem from two practical points of view although it becomes difficult to obtain a clear, reconciled understanding. In the first approach, one either makes a numerical solution of Hartree-Fock equations or the Kohn-Sham equations for a few electrons and obtain the electron density. The density profile shows a typical crystal like structure consisting of hills and valleys\textsuperscript{2–4}. It is known that this is an artifact of the non linearity of the equations in use while the exact theory is linear\textsuperscript{6}. In the other approach, one makes an exact diagonalization for even fewer electrons. Whereby, the density do not show any signature of broken symmetry because of the linear superposition principle. However if one calculates the pair correlation function, then that shows oscillations\textsuperscript{4,7,8}. Generally speaking, these oscillations survive over a finite length and decay rapidly which is expected in finite size systems. The correlation function is not defined in Hartree-Fock Theory or Density Functional Theory. The density oscillations obtained therein do not decay beyond a length scale. Still one makes the ad hoc assumption that the non linearity of Hartree-Fock Theory or Density Functional Theory show density oscillations by projecting the pair correlation function and consequently, the discrepancy of the decay disappears for infinite systems. With exact diagonalization, one also looks at the degeneracy of eigen energies after subtracting the center of mass energy and checks if the degeneracy can be explained by the representative point group corresponding to the broken
FIG. 1: (a) Yrast spectra for electrons in a one dimensional ring. The electrons are interacting only through statistics whence Coulomb interaction is ignored. The circles and the stars are the calculated data points. The circles are for 8 spin up electrons (connected by dotted line) and the stars are for 4 spin up and 4 spin down electrons (connected by dash-dot line). The solid line is drawn by connecting the local minima of the 8 spin up electrons and dashed line is drawn connecting the local minima for the 4 spin up 4 spin down electrons. The solid and dashed line fall on a parabola given by $M^2/2I$ where $M$ is the total angular momenta and $I$ is the moment of inertia for 8 classical particles in a one dimensional ring. (b) The energy values are plotted after subtracting solid and dashed line in Fig. 1a from dotted and dash-dotted lines, respectively, in Fig. 1a.

Symmetry crystalline state. Once again, one cannot go to very large energy limits due to numerical problems. Already at higher energies one starts to notice deviations from exact degeneracies just as oscillations in pair correlation function decay beyond a certain length scale.

Mesoscopic systems give a unique opportunity to study the few electron system both experimentally as well as with theoretical models and hence provide an opportunity to study how few electron properties evolve into macroscopic collective properties as we increase the number of electrons. Wigner crystallization of electrons, one such bulk phenomenon of spontaneous symmetry breaking proposed long ago, is still a debatable issue. We exclude here the situation when quantum mechanical kinetic energy or the uncertainty of an electron can be quenched by a strong magnetic field or the situation when explicit symmetry breaking leads to an electron crystal state.
II. ONE DIMENSIONAL RING

In one dimension, correlation due to Pauli exclusion principle alone can cause oscillation in pair correlation function within short distances even in absence of Coulomb interaction. One dimensional system however, is an idealization that is well understood. If one takes a finite number of electrons in a one dimensional ring, the eigen energy can be calculated very easily. A typical curve is shown in Fig. 1. The structure obtained in Fig. 1 can be understood in terms of spontaneous symmetry breaking. The electrons form a crystal in the center of mass frame while the center of mass behaves like a free particle and hence the solid and dashed curve in Fig. 1 increases parabolically. The points B and C correspond to excitations that are therefore decoupled from the center of mass motion and corresponds to vibrations of localized electrons in center of mass frame. If the parabolic contribution is subtracted then the yrast spectra show periodic oscillation (Fig. 1b). That is, if one subtracts the solid line from circular dots in Fig. 1a, one gets the dotted line in Fig. 1b and if one subtracts the dashed line from the stars in Fig. 1a, one gets the dash-dot line in Fig. 1b. Figs. 1a and 1b imply that eight spin up electrons, crystallized in a one dimensional ring has eight-fold discrete symmetry while four up and four down has a four-fold discrete symmetry. Hence the yrast spectrum repeats modulo eight and four respectively in Fig. 1b. As the length of the ring tends to infinity the points B and C in Fig. 1a will come closer to the point A and we get Fig. 1 of Ref. [18]. Such an infinite one dimensional system can be bosonized wherein the bosonic excitations are the above mentioned vibrations of localized charge that act as phonons. This is well studied using Luttinger liquid, Calogero-Sutherland model and Bethe Ansatz. Two dimensional systems are not very well understood although there have been lot of efforts to show the same features in two dimensions due to the experimental observations in heavy fermion systems and high temperature superconductors. In this paper, we wish to show that quasi one dimensional system can provide very interesting clue to understand the corresponding higher dimensional analogues as well.

III. QUASI ONE DIMENSIONAL RING AND TWO DIMENSIONS

Let us consider N number of electrons in a quasi one dimensional (Q1D) ring. The Hamiltonian in presence of a magnetic field perpendicular to the plane of the ring is given
by

\[ H = \sum_{j=1}^{N} \left[ \frac{1}{2m^*} \left( -i\hbar \nabla_j - \frac{e}{c} \vec{A}(\vec{r}_j) \right)^2 + V(r_j) \right] + \frac{1}{2} \frac{1}{4\pi e} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \]  

(1)

where \( V(r_j) \) is the confinement potential for jth electron defined as

\[ V(r_j) = \begin{cases} 0 & \text{for } r_{in} \leq r_j \leq r_{out} \\ \infty & \text{elsewhere} \end{cases} \]  

(2)

Here \( r_{in} \) is the inner radius and \( r_{out} \) is the outer radius of the ring. We use a unit system where \( \hbar = 1, \ c = 1, \ e = 1, \ 4\pi\epsilon_0 = 1 \) and \( m^* = 0.5 \) and we choose the Bohr radius \( (\frac{4\pi\epsilon_0\hbar^2}{m^*e^2}) \) to be the unit of length. Such a Q1D ring can be experimentally realized.\(^{22}\)

A. Single particle states

Single particle Hamiltonian \( (H_0) \) in presence of a magnetic field is given by disregarding the last term in Eq. (1) and the sum in the first term. Therefore, the index \( j \) is dropped. The corresponding Schrödinger equation is

\[ \left[ \frac{1}{2m^*} \left( -i\hbar \nabla - \frac{e}{c} \vec{A} \right)^2 + V(r) \right] \psi = E\psi \]  

(3)

We use two dimensional polar coordinates \( (r, \theta) \). The vector potential in Coulomb gauge \( (\nabla \cdot \vec{A} = 0) \) is given by

\[ \vec{A}(\vec{r}) = \frac{Br_f^2}{2r} \theta = \frac{\omega_c m^* r_f^2}{2er} \hat{\theta} \]  

(4)

where \( B \) is the magnetic field passing through a finite circle of radius \( r_f < r_{in} \) and \( \omega_c = (eB/m^*c) \) is the cyclotron frequency. The above equation can be solved\(^{23,24}\) and we outline below our solution as our boundary conditions are different. Thus from Eq. (3) and Eq. (4),

\[ \frac{1}{2m^*} \left[ -\hbar^2 \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) - \frac{\hbar^2}{r^2} \frac{\partial^2}{\partial \theta^2} + i (\hbar m^* \omega_c r_f^2) \frac{\partial}{\partial r} + \left( \frac{m^* \omega_c r_f^2}{2} \right)^2 \frac{1}{r^2} + V(r) \right] \psi = E\psi \]  

(5)

Let us consider the region within the ring \( (r_{in} \leq r \leq r_{out}) \) where the potential \( V(r) \) is zero. Multiplying both sides by \( \frac{2m^*r^2}{\hbar^2} \), we get from Eq. (5),

\[ \left[ \frac{r}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{2m^*E}{\hbar^2} - \left( \frac{m^* \omega_c r_f^2}{2\hbar} \right)^2 \right] \psi + \left[ -i \frac{m^* \omega_c r_f^2}{\hbar} \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} \right] \psi = 0 \]  

(6)
Eq. (6) allows us to write
\[ \psi(r, \theta) = R(r)\Theta(\theta) \] (7)

Thus from Eq. (6) and Eq. (7) we get
\[ r \frac{d}{dr} \left( r \frac{dR}{dr} \right) + \left( \frac{2m^*E}{\hbar^2} r^2 - \alpha^2 - \lambda \right) R = 0 \] (8)
\[ \frac{d^2\Theta}{d\theta^2} - i2\alpha \frac{d\Theta}{d\theta} + \lambda \Theta = 0 \] (9)

where \( \lambda \) is a separation constant and \( \alpha \) is given by
\[ \alpha = \frac{m^*\omega_0 r^2}{2\hbar} = \frac{\Phi}{\Phi_0} \] (10)

\( \Phi \) is the flux passing through the ring and \( \Phi_0 \) is the flux quantum given by \( \frac{eh}{c} \). Solution for Eq. (9) is given by
\[ \Theta(\theta) = \frac{1}{\sqrt{2\pi}} e^{x} \left[ e^{i(\alpha \pm \sqrt{\alpha^2 + \lambda}) \theta} \right] \] (11)

The azimuthal wave function \( \Theta(\theta) \) satisfy twisted periodic boundary condition, i.e., \( \Theta(\theta) = \Theta(\theta + 2\pi) e^{-\frac{2\alpha \phi}{\Phi_0}} \) that gives
\[ \alpha \pm \sqrt{\alpha^2 + \lambda} = \alpha \pm m' \] (12)

where, \( m' = \sqrt{\alpha^2 + \lambda} = 0, \pm 1, \pm 2, \ldots \)

Hence,
\[ \Theta(\theta) = \frac{1}{\sqrt{2\pi}} e^{x} \left[ e^{i(\frac{\phi}{\phi_0} \pm m') \theta} \right] \] (13)

Let
\[ x' = \sqrt{\frac{2m^*E}{\hbar^2} r} = kr \] (14)

Using Eq. (14) in Eq. (8) one gets the Bessel’s equation of first kind given by
\[ x'^2 \frac{d^2R}{dx'^2} + x' \frac{dR}{dx'} + \left( x'^2 - m'^2 \right) R = 0 \] (15)

The solution of Eq. (15) is given by
\[ R(r) = A_{m'} J_{m'} (kr) + B_{m'} N_{m'} (kr) \] (16)

where \( J_{m'} \) and \( N_{m'} \) are the Bessel and Neumann function of order \( m' \). The boundary conditions for the radial function \( R(r_{in}) = R(r_{out}) = 0 \) gives
\[ \frac{-A_{m'}}{B_{m'}} = \frac{N_{m'} (k r_{in})}{J_{m'} (k r_{in})} = \frac{N_{m'} (k r_{out})}{J_{m'} (k r_{out})} \] (17)
\[ N_{m'} (k r_{in}) J_{m'} (k r_{out}) = N_{m'} (k r_{out}) J_{m'} (k r_{in}) \] (18)
Eq. (18) determines the allowed values of energy for a particular \( m' \). So the complete solution can now be written by combining Eqs. (16) and (13) as,

\[
\psi(r, \theta) = \left[ (A_{m'} J_{m'}(k_n r) + B_{m'} N_{m'}(k_n r)) \exp \left( i(m' + \frac{\Phi}{\Phi_0}) \theta \right) \right] \quad (19)
\]

\( k_n \) should be defined as \( E_n = \frac{\hbar^2 k_n^2}{2m^*} \). Note that there seems to be no obvious decoupling of the radial part and the azimuthal part in \( \Psi(r, \theta) \). The eigen energy cannot be expressed as a sum of two terms and the total energy has to be found by solving Eq. (18). But if we solve Eq. (18) numerically and plot the eigen energies then the radial and the azimuthal part appears to get decoupled. This is shown for \( n = 1, \) and \( n = 2 \) in Fig. 2. Possible \( m' \) values corresponding to a particular \( n \) value form a distinct band signifying decoupling of radial energy and azimuthal energy. Each curve is a parabola for both \( n = 1 \) and \( n = 2 \) just like what we get in a one dimensional ring.

We can get further insight when we move into higher dimensions by noting the similarities between Q1D and 1D. Multiplying both sides of Eq. (8) and Eq. (9) by \( \frac{\hbar^2}{2m^*} \) and adding...
- $\frac{m^* \omega^2 r_f^2}{8r^2}$ to both sides of Eq. (9) one can obtain the following equations

$$-\frac{\hbar^2}{2m^*} \frac{1}{r} \frac{d}{dr} \left( r \frac{dR}{dr} \right) + \left( \frac{m^* \omega^2 r_f^2}{8r^2} + \frac{\lambda \hbar^2}{2m^* r^2} - E \right) R = 0 \tag{20}$$

$$\frac{1}{2m^*} \left( \hat{p}_\theta - \frac{e}{c} A(r) \right)^2 \Theta(\theta) = \left( \frac{m^* \omega^2 r_f^2}{8r^2} + \frac{\lambda \hbar^2}{2m^* r^2} \right) \Theta \tag{21}$$

where, $\hat{p}_\theta = -i\hbar \frac{\partial}{\partial \theta}$.

If we write,

$$E_1(r) = E - \frac{m^* \omega^2 r_f^2}{8r^2} - \frac{\lambda \hbar^2}{2m^* r^2} = E - \frac{\hbar^2 m'^2}{2m^* r^2} \tag{22}$$

then Eq. (20) reduces to a simple form

$$-\frac{\hbar^2}{2m^*} \left[ \frac{1}{r} \frac{d}{dr} \left( r \frac{dR}{dr} \right) \right] R(r) = E_1(r) R(r) \tag{23}$$

Using Eq. (23) in Eq. (21), we further obtain

$$\frac{1}{2m^*} \left( -i\hbar \frac{1}{r} \frac{\partial}{\partial \theta} - \frac{e}{c} A(r) \right)^2 \Theta(\theta) = (E - E_1(r)) \Theta(\theta) \tag{24}$$

Since $rd\theta = dx$, Eq. (24) becomes

$$-\frac{\hbar^2}{2m^*} \left( \frac{d}{dx} - \frac{ieA(r)}{\hbar} \right)^2 \Theta(x) = [E - E_1(r)] \Theta(x) \tag{25}$$

$\Theta$ which is a function of $m'$ and $\theta$ in Eq. (24) now becomes a function of $k$ and $x$ in Eq. (25).

The $r$ dependence of $A$ is of no consequence as $A(r)$ in Eq. (25) can be gauged away in a manner just as one does in the 1D case to give

$$-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \Theta'(x) = [E - E_1(r)] \Theta'(x) \tag{26}$$

where $\Theta'$, the gauge transformed version of $\Theta$ is given by

$$\Theta'(x) = \Theta(x) e^{-\frac{i}{\hbar} \int_{0}^{r} A(r) r d\theta} \tag{27}$$

Ref. [25] writes for a one dimensional ring

$$-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \Theta'(x) = E_{1D} \Theta'(x) \tag{28}$$

Note that Eq. (26) and Eq. (28) give similar energy spectrum as has already been clearly explained in Fig. 2. $E - E_1(r)$ in Eq. (26) corresponds to $E_{1D}$ in Eq. (28). Only
FIG. 3: Probability distribution of radial wave function of an electron in a ring with (a) $r_{in} = 8R_B$, $r_{out} = 12R_B$ and (b) $r_{in} = 4R_B$, $r_{out} = 12R_B$ for different $m'$ values. In (a) all the curves corresponding to different $m'$ values overlap on each other but in (b) they are distinct (here we have shown for $m'=0$, $m'=4$, $m'=6$). Situation in (a) leads to a broken symmetry state and for (b) symmetry is restored.

The difference is that $[E - E_1(r)]$ in Eq. (26) has to be determined from Eq. (23) and the radial wave function compensates in such a way that the eigen energies of the system turn out to be similar in quasi one dimension as well as in one dimension. This is true for a narrow ring as well as a wide ring. A gradual crossover to an extremely wide ring that can be considered as a two dimensional system does not change this feature. The only change of feature will be in the nature of the radial wave function. This is well demonstrated in Fig. 3 where, the probability density is plotted across the radius of the ring for different $m'$ values corresponding to $n=1$. For narrow rings, the wave functions corresponding to possible different $m'$ values look identical. However, for wider rings this is not true; for two different $m'$ values there is a lot of difference in the wave function profile. We have plotted only for a few values of $m'$ just for the sake of visual clarity of the figures.

B. Effect of Fermi Statistics

In Fig. 4a we consider the same parameters as are used in Fig. 2a and plot the yrast spectra for (i) 8 up spin electrons (plotted as circles) and (ii) 4 up, 4 down (plotted as stars) spin electrons. Note that, we are not including the effect of Coulomb interaction but consider the consequences of Fermi statistics only. The dash-dot line and the dotted line are guides to the eye. It can be seen clearly that, we obtain an identical behaviour in quasi one dimension (Fig. 4a) as compared to in one dimension depicted in Fig. 1a. This demonstratively
signifies decoupling of the center of mass energy and the energy associated with the internal degrees of freedom. This in turn, implies the breakdown of symmetry in the internal frame as has already been explained along with Fig. 1a. We see that, the local minima increases parabolically with the magnitude of flux exactly as it happens in a one dimensional ring. We fit the local minima to $M'^2/2I$, where $M'$ is the designated total angular momentum which has been calculated quantum mechanically i.e. using the relation, $M' = \Sigma m'_i$. We have used $I$, the moment of inertia as a fitting parameter and have obtained the value of $I$ to be $791.4 \ m_eR_B^2$ for a ring of inner radius $8R_B$ and outer radius $12R_B$. The moment of inertia for 8 classical electrons placed at equal distances in a ring like arrangement and rotating on a ring of radius $10R_B$ is $800 \ m_eR_B^2$. This further confirms a semi rigid classical structure and hence symmetry breaking. In Fig. 4b, where like in Fig. 1b, we have used the same procedure of subtracting the original data from the parabolic line. The perfect periodicity of a broken symmetry state is again clear from the periodicity of the current (modulo 8 and 4).
FIG. 5: Change in periodicity with variation of thickness for a ring with 8 spin up electrons. Here $r_{in} = 4R_B$ and $r_{out} = 12R_B$. (a) Yrast spectra of the ring. Circles are the exact data points which are connected by dotted line and the minima are connected by a solid line. (b) Energy spectra after subtracting the solid line from the dotted line in (a). The periodicity is broken unlike in Fig. 4.

We will now show that in quasi one dimension unlike in one dimension there can be a transition that can be effected by increasing the thickness of the ring. Hence we plot the yrast spectra (Fig. 5a) for a ring of inner radius $4R_B$ and outer radius $12R_B$. We subtract the parabolic data from the original data and plot the resulting value. It is not exactly periodic as can be seen in Fig. 5b. The periodicity is destroyed for larger $M'$ (Fig. 5b). We again fit the local minima to $M'^2/2I$ using $I$ as fitting parameter. The value of $I$ we obtain from the fitting is 551.8 $m_eR_B^2$. The moment of inertia for 8 classical electrons sitting at equal distance in a ring like arrangement and rotating on a circle of radius $8R_B$ is 512.0 $m_eR_B^2$. Hence in this case we can’t say that the particles are behaving almost as classical particles which are localized at equal distances in the center of mass frame. In one dimension, statistics plays a major role as the particles can not cross each other. In a two dimensional ring with inner radius $8R_B$ and outer radius $12R_B$, we see that the radial probability distribution for all $m'$ values coincide with each other (Fig. 3a). In this case, it looks like the effect is similar to the case of one dimension and that the particles can not cross each other. For a ring of inner radius $4R_B$ and outer radius $12R_B$ the position of peaks of the radial probability distribution changes with $m'$ (Fig. 3b). In this case it appears that unlike in 1D the particles can cross each other inside the ring.
FIG. 6: Periodicity is restored when the radius and thickness are changed simultaneously. Stars are data for $r_{in} = 4R_B$ and $r_{out} = 6R_B$, and circles are data for $r_{in} = 8R_B$ and $r_{out} = 12R_B$ for a ring with 16 spin up electrons.

From Fig. 5 and associated narrations, it seems that symmetry breaking is not possible in two dimensions that can be obtained by gradually increasing the thickness of a Q1D ring. But if we increase the radius and the thickness simultaneously, it results in a symmetry breaking as we will explain now. We take 16 electrons interacting only due to Fermi statistics and compare the energy spectra for two rings. One with inner radius $4R_B$ and outer radius $6R_B$ and another with inner radius $8R_B$ and outer radius $12R_B$. Here we have not plotted the yrast spectra, but plotted the energy values after subtracting the parabolic data we obtain by connecting the minima (Fig. 6). We see that both the curves show the same periodicity signifying broken symmetry. The amplitude of energy for the ring with inner radius $8R_B$ and outer radius $12R_B$ is $1/4$-th of the amplitude for the ring with inner radius $4R_B$ and outer radius $6R_B$. This is also similar to the case of a one dimensional ring, where if one makes the radius double, the energy becomes $1/4$-th. Hence it seems quite natural that, by increasing the radius and the thickness simultaneously one can observe symmetry breaking for an infinite two dimensional system as well. This is because the act of increasing the radius consequently lowers the azimuthal component of the momentum and the act of increasing the thickness lowers the radial component of the momentum. Thus it seems that even in 2D, one can find very low energy states with a broken symmetry.
C. Effect of Coulomb Interaction

Wave function for the Hamiltonian in Eq. (1) can be written in terms of \( \psi(r, \theta) \) of Eq. (19) as the many particle extension

\[
\Psi_N(\{r_j, \theta_j\}) = \sum a\{m'_j\} \mathcal{A} \prod_{j=1}^{N} \left( (A_{m'_j}J_{m'_j}(k_n r_j) + B_{m'_j}N_{m'_j}(k_n r_j)) \left( \frac{1}{\sqrt{2\pi}} e^{im'_j \Phi / \Phi_0} \theta_j \right) \right)
\]

(29)

where \( a\{m'_j\} \)s are unknown coefficients. \( \{m'_j\} \) corresponds to the set of all allowed \( m'_j \) values.

We now introduce the center of mass (\( \xi \)) and relative (\( \zeta_i \)) coordinates defined as

\[
\xi = \frac{1}{N} \sum_{j=1}^{N} \theta_j
\]

(30)

\[
\zeta_j = \theta_j - \xi
\]

(31)

The many body Hamiltonian (Eq. (1)) in terms of the center of mass and the relative coordinates is given by

\[
\mathbf{H} = \sum_{j=1}^{N} \frac{-\hbar^2}{2m^* r_j^2} \frac{1}{N^2} \frac{\partial^2}{\partial \xi^2} + \sum_{j=1}^{N} \left( \frac{-\hbar^2}{2m^*} \frac{1}{r_j} \frac{\partial}{\partial r_j} \left( r_j \frac{\partial}{\partial r_j} \right) + V(r_j) \right)
\]

\[
+ \sum_{j=1}^{N} \frac{-\hbar^2}{2m^* r_j^2} \frac{\partial^2}{\partial \zeta_j^2} + \sum_{j=1}^{N} \frac{-\hbar^2}{2m^* r_j^2} \frac{1}{N^2} \left( \sum_{k=1}^{N} \frac{\partial}{\partial \zeta_k} \right)^2
\]

\[
+ \sum_{j=1}^{N} \frac{2}{N^2} \frac{-\hbar^2}{r_j^2} \frac{\partial}{\partial \zeta_j} \left( \sum_{k=1}^{N} \frac{\partial}{\partial \zeta_k} \right) - \sum_{j=1}^{N} \frac{2}{N^2} \frac{-\hbar^2}{r_j^2} \frac{\partial}{\partial \zeta_j} \sum_{k=1}^{N} \frac{\partial}{\partial \zeta_k} - \sum_{j=1}^{N} \frac{2}{N^2} \frac{-\hbar^2}{r_j^2} \frac{\partial}{\partial \zeta_j} \sum_{k=1}^{N} \frac{\partial}{\partial \zeta_k}
\]

\[
+ \frac{1}{2} \sum_{i \neq j} \frac{1}{4\pi \epsilon} \frac{e^2}{\sqrt{r_i^2 + r_j^2 - 2r_i r_j \cos(\zeta_i - \zeta_j)}}
\]

(32)

Here, \( N \) is the total number of electrons.

Our non-interacting calculations suggests that in some regime if \( r_j = \text{constant} = r_{1D} \)
then the first term in Eq. (32) is \( \hat{M}'^2 / 2I \) where \( \hat{M}' = -i\hbar \frac{\partial}{\partial \xi} \) and \( I = m^* N r_{1D}^2 \). Note \( -i\hbar \frac{\partial}{\partial \xi} \) commutes with \( \mathbf{H} \) in Eq. (32). This essentially implies that Coulomb interaction (the last term) will not change the center of mass angular momentum and hence \( \sum m'_j = M' \) (where \( M' \) is the eigenvalue corresponding to \( \hat{M}' \)) will be a conserved quantity. Its value remains the same whether the last term in Eq. (32) is included or not. Therefore, substituting for \( \theta_j \) from Eq. (30) and Eq. (31) in Eq. (29)
\[
\Psi(\{r_j, \theta_j\}) = e^{i(M' + N \frac{\Phi_0}{\Phi_0})} \sum_{\{m'_j\}} \xi \prod_{j=1}^{N} \left[ \left( A_{m'_j} J_{m'_j} (k_n r_j) + B_{m'_j} N_{m'_j} (k_n r_j) \right) \right]
\]
\[
\left( \frac{1}{\sqrt{2\pi}} e^{im'_j \zeta_j} \right)
\]
(33)

This is because if we switch off the Coulomb interaction then the sum will not appear in the
wave function and hence, the exact wave function is
\[
\Psi(\{r_j, \theta_j\}) = e^{i(M' + N \frac{\Phi_0}{\Phi_0})} \xi \prod_{j=1}^{N} \left[ \left( A_{m'_j} J_{m'_j} (k_n r_j) + B_{m'_j} N_{m'_j} (k_n r_j) \right) \right]
\]
\[
\left( \frac{1}{\sqrt{2\pi}} e^{im'_j \zeta_j} \right)
\]
(34)

This argument can be given for each term in the sum of Eq. (33). So note that the flux
dependence remains the same in presence or absence of Coulomb interaction. This is because
the term inside the summation in Eq. (33) does not contain flux and the periodicity will be
\(\Phi_0/N\) as can be seen from Eq. (34) provided we start from the periodic structure as in Fig.
4. If we do not start from a periodic structure then the \(N\Phi/\Phi_0\) in the exponent of Eq. (33)
does not imply a \(\Phi_0/N\) periodicity. Aharonov-Bohm effect in a ring can be observed\textsuperscript{26}. So
changes in periodicity can also be observed and can give us the demonstration of symmetry
breaking transition.

IV. THREE DIMENSIONS

![FIG. 7: A three dimensional ring](image)

For a three dimensional ring (shown in Fig. 7), the single particle Schrödinger equation
is given by
\[
\left( -\frac{\hbar^2}{2m^*} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] + V(r, \theta, \phi) \right) \Psi = E\Psi
\]
(35)
where the potential is defined as

\[ V(r, \theta, \phi) = 0 \quad \text{inside the shaded region} \]

\[ = \infty \quad \text{everywhere else} \quad (36) \]

If we express the total as \( \Psi = R(r)P(\theta, \phi) \) then Eq. \( (35) \) becomes

\[- \frac{1}{R} \left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{2m^*r^2}{\hbar^2} V(r) + \frac{2m^*r^2E}{\hbar^2} \right\} R(r) = \frac{1}{P} \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right\} P(\theta, \phi) \quad (37)\]

If \( \theta \) is very small then \( \sin \theta = \theta \) and Eq. \( (37) \) becomes

\[- \frac{1}{R} \left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{2m^*r^2}{\hbar^2} V(r) + \frac{2m^*r^2E}{\hbar^2} \right\} R(r) = \frac{1}{P} \left\{ \frac{1}{\theta} \frac{\partial}{\partial \theta} \left( \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\theta^2} \frac{\partial^2}{\partial \phi^2} \right\} P(\theta, \phi) = \lambda \quad (38)\]

Once again the radial part effectively decouples and one can have

\[ \left\{ \frac{1}{\theta} \frac{\partial}{\partial \theta} \left( \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\theta^2} \frac{\partial^2}{\partial \phi^2} \right\} P(\theta, \phi) = \lambda P(\theta, \phi) \quad (39)\]

If we replace \( \theta \) by \( r \), then Eq. \( (39) \) will look identical to Eq. \( (5) \) in absence of magnetic field. Magnetic field and Coulomb interaction can then be treated in the same way as we have done for Eq. \( (5) \). In such a ring therefore the equation of motion is just like in 1D and hence we can again expect symmetry breaking. However, if \( \sin \theta \) can not be approximated by \( \theta \) then we should not expect symmetry breaking in three dimensions. Thus we cannot get symmetry breaking in atoms.

V. CONCLUSIONS

We show that in quasi-one-dimension and two dimensions, owing to internal symmetry breaking transition can take place for a many electron state. In the broken symmetry state, the electrons crystallize in the internal frame and behave like a semi-rigid rotor. The low-lying excitations are associated with rotations and vibrations of this semi-rigid rotor. While it is known that one-dimensional systems always show a broken symmetric state and no transition, the broken symmetry state in Q1D is identical to that in 1D and the transition is unique to Q1D and 2D. In three dimensions however, it is unlikely that a broken symmetric state can exist. One can experimentally verify the broken symmetry state by taking a ring made up of the Q1D wire and generating a persistent current in the ring. The flux periodicity
of the persistent current gives the signature of a broken symmetry state. When the system becomes like a semi-rigid rotor, the flux periodicity becomes $\phi_0/N$, where $N$ is the number of electrons in the ring. In the symmetric state, the $\phi_0/N$ periodicity is destroyed. In finite systems, the transition is always gradual as is generally expected.

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