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ELECTRONS IN A MAGNETIC FIELD, WIGNER CRYSTAL AND THE FRACTIONAL QUANTUM HALL EFFECT

A Thesis submitted for the Degree of
Doctor Philosophiae

Academic Year 1990-91

Candidate

Fabio Bagarello

Supervisor

Prof. F. Strocchi

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INTRODUCTION

In the last ten years the attention of a larger and larger number of physicists has been captured by two-dimensional systems. The main reason for this is that many new physical phenomena take place only in such systems. High-Tc superconductivity and the quantum Hall effect are typical examples of such processes. Although we are in the area of Many-Body Quantum Mechanics also those people whose interest is more oriented towards High-Energy Physics have started to look at some two-dimensional devices and to built up theoretical models for the above phenomena.

Such an interest, in our opinion, follows from the appearance of a new kind of elementary particles that do not live in the usual three-dimensional world: the anyons. These particles are characterized by the peculiarity of having not necessarely integer or half integer values of the spin. Of course the presence of such particles is strictly related to the two-dimensional nature of the samples where they are confined. The reason is that, for instance, in more than two spatial dimensions, locality forces the particles to be either bosons or fermions. The above result, known as the Spin-Statistic Theorem, strictly forbids the existence of the anyons in 3+1 dimensions.

The particular system we are interested in is a gas of electrons in a two-dimensional layer. The electrons are subjected to a strong magnetic field perpendicular to the plane.

Our interest is two-fold; first, we develop a perturbative Hartee-Fock calculation of the ground state energy. This with the aim of formalizing some results already present in the literature that, in our opinion, require more investigations. In the same perspective we will discuss some possible improvements of the energetic computation based on a single Slater determinant. Second, we will discuss some general results, both perturbative and non-perturbative, on the localization of the single-electron wave function. Its interplay with the orthogonality requirement of the translated wave functions is also discussed. The interest on localizability comes from the following natural picture of the model: due to the Coulomb interaction the electrons tend to stay far apart. Therefore the energy of the system is, in principle, lowered if the wave functions of the

electrons are 'strongly' localized around the sites of the lattice. This is the main reason why the classical result for the ground state energy, the Wigner energy, is a variational lower bound. The above guess explains why, in our opinion, it is relevant to study the maximum localization allowed to the wave function of an electron in our sample. Furthermore, we believe that orthogonality is a crucial requirement for our model, so that we also want to maintain this property. We will show that there is a strict connection between both the requirements: maximum localization and orthogonality.

We end this thesis with some notes on a possible spin model that could reproduce the physics of the two-dimensional electron gas. In particular we suggest an heuristic procedure to obtain an approximated Hamiltonian for the electrons expressed in terms of spin variables and we discuss its validity for small fillings. The spin model proposed is described by an Ising Hamiltonian with a long range interaction.

CHAPTER 1 : THE FRACTIONAL QUANTUM HALL EFFECT

1.1 : Experimental Aspects

The Quantum Hall Effect (QHE) has been observed for two dimensional electron systems at low temperatures and subjected to strong magnetic fields perpendicular to the surface of the sample, [1]. The electrons are trapped in a thin layer (about 100 Å) at the interface between semiconductors or between semiconductor and insulator. The mostly used devices in observing QHE are Si MOSFET (*Metal- Oxide- Semiconductor- Field- Effect- Transistor*) and GaAs-AlGaAs heterojunction.

Typically for the integer QHE (IQHE), the temperature range is $T \approx 1-4$ °K and the magnetic field is about $B \approx 3-15$ Tesla. For the fractional QHE (FQHE) the temperature is even lower: $T \approx 20-100$ °mK and the magnetic field needs to be stronger: $B \approx 15- 30$ Tesla.

The data are normally presented as two curves: ρ_{xy} versus B and ρ_{xx} versus B. Here we suppose that an electric field is applied in the y-direction and the Hall current is in the x-direction. $\rho_{xx} = V_x / I_x$ and $\rho_{xy} = V_y / I_x$ are, respectively, the longitudinal and transverse resistance.

The basic feature of the experimental curves (see fig. 1 below) is the appearance of the Hall resistance plateaus at filling near all low-lying integers, $\nu = 1,2,3,...$, and near some special fractions such as 1/3, 2/3, 1/5, 2/5,..... . Corresponding to the plateaus in ρ_{xy}, there are valleys in ρ_{xx} with $\rho_{xx} \approx 0$ or at least sharp dips in ρ_{xx} . When ρ_{xx} is zero the inverse of ρ_{xy} gives the Hall conductance σ_{xy}.

Another remarkable feature of the QHE is that at the plateaus the Hall conductance is quantized to take the value

$$\sigma_H \equiv \rho_{xy}^{-1} = \nu \frac{e^2}{h}$$

Depending on ν being integer or fractional we call the effect IQHE or FQHE. We observe that the curves have similar features in both cases. However the FQHE corresponds to partially filled Landau levels, while the IQHE is related to totally filled levels. The parameter ν is essentially the density of the two-dimensional electron gas, and it gives the number of electrons per quantum flux. The number of electrons per unit area is

usually fixed in heterojunctions, and ν can be modified by changing the magnitude of the magnetic field.

The third feature, which makes the QHE practically useful and scientifically fascinating, is the high accuracy with which the quantization of σ_H has been observed: $\Delta\nu \leq 10^{-8}$ for the IQHE, and $\Delta\nu \leq 10^{-5}$ for the FQHE.
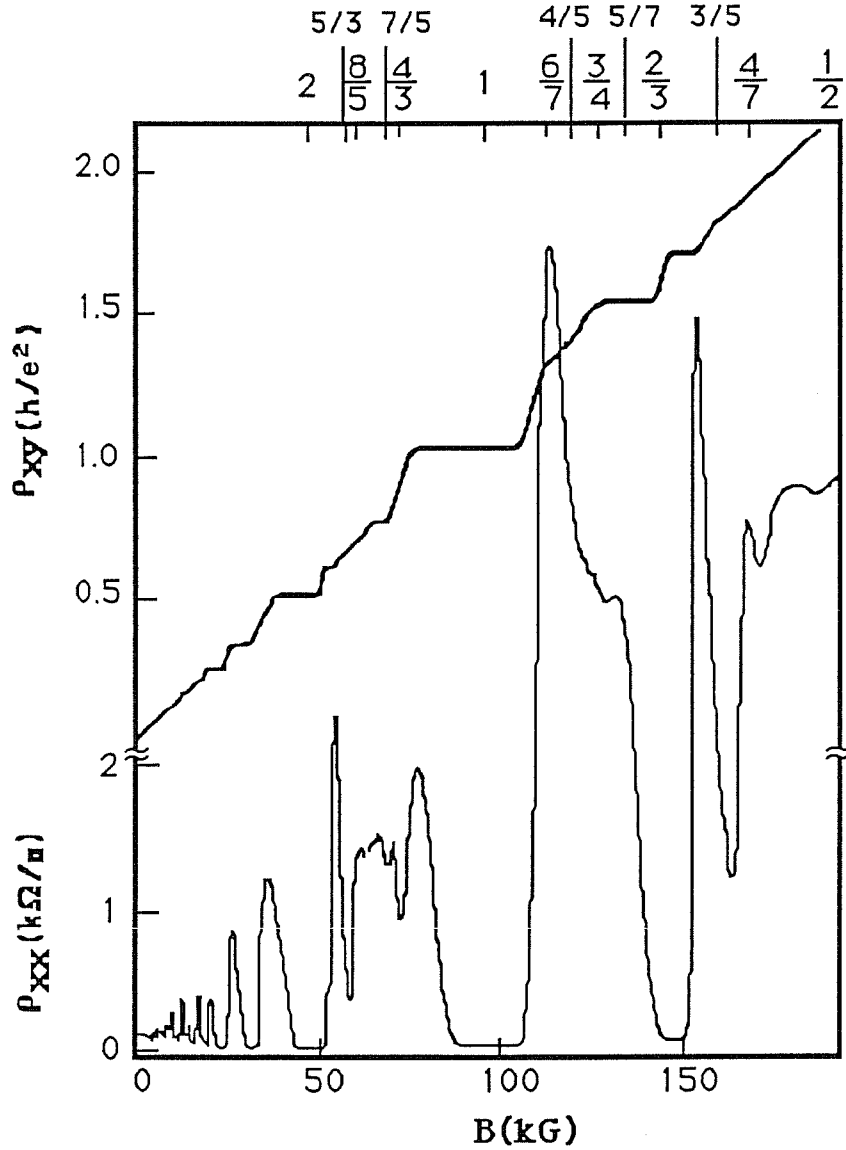

Fig. 1

A crucial rôle in both theoretical and experimental QHE is played by the impurities in the sample: in a model in which the potential describing such impurities is strong compared to the Coulomb interaction between electrons, the effect is destroyed. In the opposite conditions such impurities, by localizing the charges in the sample, facilitate observation of

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the effect. The border between the two regimes is still delicate and controversial, [2].

All throughout this work we will restrict to a clean sample, neglecting the effects of any impurities. A general discussion of the effects of the impurities in the QHE can be found, for instance, in reference [2].

1.2: Ground State: a review

The physical model we have in mind consists in an electron gas with no impurity in a uniform positive background. This system has been widely discussed in the past years and even nowadays it is often subject of new studies and researches. The first 'modern' approach to this system is due to Wigner in 1934, [3]. He studied a homogeneous electron gas in a neutralizing positive charge. He pointed out that the behaviour of such a gas as a function of the particle density is very different from that of a gas of classical particles. In a classical gas, one expects that the lower the particle density is, the less important will be the interparticle interactions for the properties of the gas. By contrast, in the electron gas the Coulomb interaction becomes more important the smaller the density is, so that a high-density electron gas behaves almost like an ideal gas of fermions. Wigner argued that below a certain critical density the kinetic energy will be negligible and the behaviour of the gas will be determined by which electron configuration minimizes the potential energy due to the Coulomb interaction. Since the potential energy of a random array is higher than that of an ordered array, he concluded that at densities smaller than some critical value the electron gas will form a crystal. In three dimensions the lowest potential energy is obtained for a body-centered cubic crystal. In 1971 R.S. Crandall and R. Williams, [4], applied Wigner's argument to a two-dimensional electron gas and concluded that such a gas will also crystallize in the low-density limit.

A further extension of Wigner's argument by Yu. E. Lozovik and V. I. Yudson in 1975, [5], showed that a two-dimensional electron gas (2DEG) will have a crystalline phase also when the system is subjected to a strong magnetic field normal to the plane of the gas. They also argued that the behaviour of such a gas becomes classical in the limit of an infinitely strong magnetic field.

Additional studies on the Wigner crystal (WC) have been developed in [6], where it is computed the classical static ground-state energy of the two-dimensional electron crystal for each of the five two-dimensional Bravais lattices: the oblique, the square, the hexagonal, the primitive rectangular and the centered rectangular lattices.

The results in [6] are applied in [7] to build up a quantum approach to the WC. We believe the results in [6] are so important essentially because, as we will widely discuss in the following, one expects that all the physically relevant quantum approaches to the 2DEG have as a limit for low densities (or, equivalently, for high magnetic field), exactly the classical WC discussed in [6]. This, of course, agrees with the guess in [5].

The relevance of the WC approach to the system is nowadays out of doubt: first, everyone agrees with the guess that at low densities the ground state is certainly a WC of electrons; therefore, due to the electron-hole symmetry of the Hamiltonian, discussed, for instance, in reference [8], the ground state for densities near to 1 must be a WC of holes. Second: in recent papers, [9], new experimental results have been exposed that go in the direction of the WC. The idea is that a crystal that is pinned to the substrate cannot move until an applied electric field exceeds a threshold value, which is a measure of the force responsible of the pinning. The current-voltage characteristics of an electron gas in the WC phase are therefore expected to be nonohmic: the conductivity is expected to be very small below a certain threshold voltage, and to rise rapidly when the voltage exceeds the threshold value. Two groups have reported seeing such behaviour, [9]. The features reported by these two groups occur both at ν a little larger than 1/5 and for ν smaller than 1/5. However the value of the threshold voltage differs in a significant way in the two experiments.

The reason why this feature has been observed only in recent days is mainly that the electron mobility in the samples used in the recent experiments is 50-100 times higher than the one of the 'old' samples. Of course the higher the electron mobility is, the easier it is to unravel new features (for example in the resistivity data).

Another reason for the WC to be so relevant is that for low densities the WC of electrons is energetically favourable. This is one of the key point that will be emphasized in the next Chapter. However, since in the WC model there is apparently no reason for some ν to be preferred, we suppose that in the WC phase no QHE has to be observed or that some new mechanism must arise to explain the stability of the related σ_H. As

Laughlin discussed in ref. [10], it is not impossible for a crystal to carry current. However, since crystals have, by definition, 'lattice position' near which the electrons have larger-than-average probability to be found, transport of electric current cannot occur without motion of the lattice as a whole, or, more precisely, by a collective excitation associated with the multiplicity of ground states. Nevertheless one would expect any impurities to break the ground-state degeneracy, pin the crystal, and prevent the electrons to carry current. Since this is not the situation of the FQHE ground state (low impurities accentuate the effect), this is not a crystal or it has extremely peculiar properties.

Many quantum properties of the WC have been discussed in [8], [11], and then in [7]. In the first two references a Charge-Density-Wave (CDW) approach is discussed. In ref. [8] a good variational energy is found but this energy turns out to be a smooth function of ν so that no cusp is obtained. In [11] the approximation is improved by considering higher harmonics of the density wave and by estimating the effect of the higher Landau levels. It turns out that either these perturbations give very small contributions that, in addition, are both smooth functions of ν. Therefore no commensuration energy is obtained considering the CDW as the ground state of the 2DEG. In [7] an equivalent approach is discussed in a certain detail: an ansatz wave function is given for the lowest Landau level. The authors prove that, neglecting the overlaps between wave functions localized around different lattice sites, which are in fact almost zero for very small density, their functions give back the same electron density

$$\rho(\underline{r}) \approx (2\pi\,l^2)^{-1} \sum_l \exp\left(\frac{-1}{2l^2}\, (\underline{r} - \underline{R}_j)^2 \right)$$

as the one exactly found in [8] and [11]. This is the reason why we say that the physical model is essentially equivalent to the one discussed by Yoshioka and Fukuyama first and by Yoshioka and Lee some years later. Obviously even Maki and Zotos do not find any commensuration energy. Nevertheless they claim that a certain commensurability can be obtained in their approach by considering the next term in the expansion of the effective potential; the drawback is that this contribution to the total energy is so small that it cannot be the source of the Hall plateaus. We believe that their approach can be significantly improved by a better

estimate of the errors and by making explicit the perturbative nature of their expansion, which is not as evident as it will be in our approach. In fact, in the expansion they use for the ground state energy, in which the n-th term contains an n-electrons interaction, it is not evident at all that the n+1-th contribution is small with respect to the n-th one so that it can be neglected. On the contrary it seems that each term of their expansion must be explicitly computed for obtaining a meaningful estimate of its value. In this way one loses the practical utility of a perturbative approach, which consists essentially in an a priori estimate of the corrections appearing in the expansion.

Another approach that strongly relies on the WC is the one developed in 1983 by Tosatti, Parrinello and Chen in [12]. However many problems arise with their method: first of all they lose from the very beginning the x-y symmetry that is a symmetry of the Hamiltonian. This is in our opinion the main reason why the values of the energy are worst than the one obtained by the CDW approach. Moreover no cusp is obtained in $E(v)$, which is still a smooth function of its variable. Therefore, as the authors themselves conclude in [13], their wave function must be a poorer version of a CDW state, since it is not variationally optimized.

In the references considered above no correlation between electrons has been introduced. In 1983 Laughlin, [14], first on the basis of exact results on the few-electrons model, see reference [10] for a general overview, proposed a Jastrow-type function, Ψ_L:

$$\Psi_L(z_1, z_2, \ldots z_N) = \left[\prod_{j<k}(z_j - z_k) \right]^m \exp\left\{ -\frac{1}{4} \sum_{i=1}^{N} |z_i|^2 \right\}$$

This function, for intermediate v, $v_0 < v < 1-v_0$, turns out to be energetically favourite. Here v_0 is a critical density to be determined.

A first remarkable feature of Ψ_L is that it allows to obtain the cusps in energy since it describes an incompressible fluid. This means that a certain amount of energy must be furnished to the system to vary a little the electron density from certain values of the form $v = n/m$, n and m being integers, so that for these peculiar values of v one observe a particular stability of the system. This stability is reflected for instance in the plateaus of ρ_{xy}. It allows also to explain the quantization of the Hall

conductance and therefore it is a good candidate for a satisfactory explanation of the FQHE. Nevertheless it has been proven by Tao in 1984, without any doubt, that Ψ_L is not the ground state of the two-dimensional electron gas system. He has shown in reference [15] that the ground state of the system with 10^{11} electrons is different from the Laughlin's wave function and that the projection of Ψ_L on the true ground state is expected to be very small. An analogous conclusion is obtained also by Laughlin himself in [14] for the case of a three electrons system.

It is now believed that a phase transition must occur at a certain critical value of the density so that the 2DEG crystallizes. What is still to debate, in our opinion, is the value of the critical density, v_o. We will come back on this point in the next Chapter.

Recently other approaches to the 2DEG have been proposed by several authors: Chui, Hakim and Ma, [16], have proposed a wave function that interpolates between the CDW and the Laughlin states. The energy for $v = 1/3$ is slightly lower than that of the fluid but, as the same authors point out, this is not a conclusive result in the direction of their ansatz wave function. In fact the justification of the Laughlin incompressible fluid wave function as a model for the $v = 1/3$ FQHE state does not simply rest on its variational energy: as first pointed out by Haldane, it is also the exact and unique ground state of a truncated model Hamiltonian representing short-range components of the interaction.

Another approach that relies on the WC was proposed in [17] by Kivelson, Kallin, Arovas and Schrieffer. They suggest that large ring exchanges in the WC can produce the required cusps in the energy at rational fractional filling factors. More explicitly, they claim that a cooperative motion of the electrons of a closed ring in the WC can produce a contribution to the partition function, and therefore to the energy, which can be orders of magnitude larger than pair exchange contributions. In addition, these contributions exhibit non-analytic cusplike behaviour for certain rational values of v.

This proposal, however, is not totally accepted: Halperin, Tesanovic and Axel in [18], agree that such an effect could occur, but they are skeptical in believing that this could be the explanation of the FQHE. Moreover, in reference [19], Thouless and Li have studied a model that, in their opinion, would suggest that no downward cusp of the ground state energy can be produced by cooperative ring exchange (CRE) processes. Actually they found an upward cusp. However in [20] Kivelson et al. show

that the argument of Thouless and Li does not apply to the strong magnetic field limit and therefore it is not conclusive.

1.3: More about the Ground State

In our opinion the Wigner approach to the 2DEG, beside having a crucial relevance by itself, is still very much to debate. The relevance was pointed out, for instance, in [9] where some experimental aspects of the 2DEG were discussed. These aspects, as the threshold voltage, clearly give an evidence for the WC, at least at low electron density (or, by the electron-hole symmetry, at high hole density). Moreover it has been already pointed out in the literature that a WC is energetically favourite for $v < v_0$. This point was extensively discussed in [21] by Levesque et al. where the ground state energies as functions of v for the CDW and for Laughlin's approaches are discussed and compared. Moreover results as the ones in [17] give some chances for WC to be also responsible for the FQHE, via a CRE mechanism. Finally, a quantum approach to WC tends to the classical WC more rapidly than the approach proposed by Laughlin. This result is implicitly contained in [21] and will be slightly modified by our results in the following Chapter.

We use a Hartee-Fock approach to the WC. Therefore it is essentially a mean field approximation of a more complex problem and, as a consequence, some features of the physical problem can be lost in our strategy. In particular no correlation between the electrons will be considered. Still, we believe that such an immediate approach can have the rôle of giving some insight on the 2DEG, and it can give a partial answer to the request in [9] for a complete quantum mechanical theory of the WC. Moreover a CRE mechanism can be thought to take place in the Wigner lattice described by our model so that this 2DEG may also be relevant for the FQHE.

We start with the one-body free Hamiltonian

$$H_0 = \frac{\Pi^2}{2M} \tag{1.1}$$

with

$$\underline{\Pi} = \underline{p} + \frac{e}{c} \, \underline{H} \wedge \underline{r} \qquad (1.2)$$

where the magnetic field is supposed to be in the z-direction. We call

$$\underline{\beta} = \frac{e}{c} \, \underline{H}$$

and we indicate by β the norm of $\underline{\beta}$, $\beta = |\underline{\beta}|$.

Many strategies for solving the above quantum mechanical problem has been discussed in the past years. In this thesis we will be concerned with two of such approaches; the first one is clearly described in [22] and it provides essentially the x-y solutions of the problem. We get in this way the eigenfunctions $\Phi_{n,m}(x,y)$. Here n and m are the quantum numbers related to the particular solution. The second approach is the one proposed by Dana, Zak et al. in a series of papers where the first step is a change of variables in Hamiltonian (1.1); see, for instance, reference [23] for a first introduction. We will describe in some details this approach in Appendix 1 and in Chapter 3 since we will use kq-representation to prove one of the results of this thesis.

In [22] the $\Phi_{n,m}(x,y)$ wave functions are derived. They have the following form

$$\Phi_{n,m}(x,y) = (2^{m+n+1}\pi \, m! \, n!)^{-1/2} \exp[\, (x^2+y^2)/4] \, \cdot$$

$$\cdot \, (\partial/\partial x + i \, \partial/\partial y)^m \, (\partial/\partial x - i \, \partial/\partial y)^n \, \exp[\, -(x^2+y^2)/2] \qquad (1.3)$$

Here and in the following we take $\hbar = M = \beta = 1$. These conditions imply also that the cyclotron frequency $\omega_c = \beta/M$ and the magnetic length $a_o = (\hbar/\beta)^{1/2}$ are both equal to one.

Since we have $H_o \, \Phi_{n,m}(x,y) = (n +1/2) \, \Phi_{n,m}(x,y)$, all the energetic levels, known as Landau levels, are degenerate in m. The lowest Landau level, that is the one with n=0, is spanned by the following set of wave functions:

$$\Phi_m(x,y) = (2^{m+1}\pi \, m!)^{-1/2} \exp[\, (x^2+y^2)/4]$$

$$(\partial/\partial x + i \, \partial/\partial y)^m \, \exp[\, -(x^2+y^2)/2] \qquad (1.4)$$

which are centered around $\underline{R} = (0,0)$ and differ each-other for the different m-depending values of $< \underline{r} >$. Of course the n=0 level is the relevant one to consider for discussing the ground state of a 2DEG.

To build up the two-dimensional crystal we also need to introduce a couple of operators that translate the wave functions along the axis of the triangular lattice we are considering. These operators have to commute with the Hamiltonian (1.1) and among themselves. This is necessary to obtain wave functions that are still eigenfunctions of H_0 and univocally defined. In [24] the construction of such operators has been widely discussed and the result is given in the form:

$$T(\underline{a}_j) = \exp\{ i \underline{\Pi}_c \cdot \underline{a}_j\} \tag{1.5}$$

where we have defined the lattice basis $\underline{a}_1$ and $\underline{a}_2$ via the

$$\underline{a}_1 = a(1,0) \qquad \underline{a}_2 = a(1/2, \sqrt{3}/2) \tag{1.6}$$

a being the lattice spacing, and $\underline{\Pi}_c$ by the formula

$$\underline{\Pi}_c = \underline{p} - \frac{e}{c} \underline{H} \wedge \underline{r}$$

In our unities $\underline{\Pi}$ and $\underline{\Pi}_c$ become:

$$\Pi_x = p_x - y/2 \qquad \Pi_y = p_y + x/2 \tag{1.7}$$

$$\Pi_{cx} = p_x + y/2 \qquad \Pi_{cy} = p_y - x/2 \tag{1.8}$$

The only non-zero commutation relations between the Π operators are:

$$[\Pi_y, \Pi_x] = [\Pi_{cx}, \Pi_{cy}] = i \tag{1.9}$$

from where it follows that

$$[H_0, T(\underline{a}_j)] = 0 \qquad j=1,2 \tag{1.10}$$

For what concerns the commutation rules between the $T(\underline{a}_j)$'s it is easily seen that the two operators commute if the following rationality condition, [24], is satisfied:

$$(\underline{a}_1 \wedge \underline{a}_2)_z = 2\pi \qquad (1.11)$$

In this hypothesis given a generic function $f(x,y)$ we can consider an uniquely defined translated function $f_{n,m}(x,y)$ by the

$$f_{n,m}(x,y) = T_1{}^n T_2{}^m f(x,y)$$

where we call $T_j = T(\underline{a}_j)$, while, if condition (1.11) does not hold, an extra over-all phase appears in the definition above, phase that depends on the path one follows to define the translated function.

Let us call

$$\Psi_{0,0}(x,y) = (2\pi)^{-1/2}\exp[- (x^2+y^2)/4] \qquad (1.12)$$

where the indexes (0,0) are related to the lattice site around which the function is localized. We see from (1.4) that $\Psi_{0,0}(x,y) = \Phi_0(x,y)$ so that $\Psi_{0,0}$ is a particular function of the first Landau level. For B high enough the various Landau levels are energetically deeply separated and therefore the Coulomb interaction can be considered as a small perturbation. In this assumption only the lowest Landau level (LLL) can be occupied by the electrons in the sample, which have not enough energy to occupy the second Landau level. More explicitly, this LLL approximation is meaningful if the spacing $\hbar\omega_c$ between Landau levels is much larger than the Coulomb repulsion between electrons $V \approx e^2/\varepsilon a$, ε being the dielectric constant. The validity of such an approximation has been investigated in [11] where it is proven that for B $\approx$ 15 T, ε =13 the correction of the higher Landau levels to the ground state energy is less than 0.8%.

We use now the T operators introduced above to built up the translated wave functions. Of course since $T(\underline{a}_j)$ commutes with the Hamiltonian it follows that

$$\Psi_{n,m}(x,y) = T_1{}^n T_2{}^m \Psi_{0,0}(x,y) \qquad (1.13)$$

are still eigenfunctions of H_0 belonging to the first Landau level, $\forall$ n,m. We can give the explicit form of the above functions:

$$\Psi_{n,m}(x,y) = (-1)^{nm}\, e^{i/2(Y_{n,m}x\, -\, X_{n,m}y)}\, \Psi_{0,0}(\underline{r}\text{-}\ \underline{R}_{n,m}) \qquad (1.14)$$

where

$$\underline{R}_{n,m} = (\ X_{n,m},\ Y_{n,m}) = -a\ (\ n+m/2\ ,\ \sqrt{3}/2\ m) \qquad (1.15)$$

is the lattice site around which the functions $\Psi_{n,m}$ are exponentially localized. We want to stress that the wave functions in (1.14) are, in our unities, essentially the same introduced by Maki and Zotos in [7], but for the factor $(-1)^{nm}$. We will discuss the utility of such a phase in Chapter 2 and in Appendix 3 were we will show that it allows an easier study of the perturbative corrections of the ground state energy. Here we only want to stress that this phase is necessary to maintain the translation invariance of the model. In fact only due to the $(-1)^{nm}$ factor we have $(\ \Psi_n, \Psi_m) = (\ \Psi_0, \Psi_{n-m})$, equality that does not hold for the single electron functions given in [7].

To simplify the notation we will use, very often, a single index to indicate the couple of integers that identifies a lattice site. For instance the functions in (1.14) will be indicated as

$$\Psi_n(x,y) = (-1)^{n_1 n_2}\, e^{i/2(Y_n x\, -\, X_n y)}\, \Psi_{0,0}(\underline{r}\text{-}\ \underline{R}_n) \qquad (1.16)$$

where, of course, we must interpret n as the pair (n_1, n_2).

In order to give to these states a precise physical meaning in view of future applications we want to orthonormalize the single-electron wave functions. In fact it is easy to verify that the overlap between two states centered at different sites is not zero but it is only exponentially decreasing. We have

$$c_n = (\ \Psi_0, \Psi_n) = \int d^2\underline{r}\ \Psi_0{}^*(\underline{r})\Psi_n(\underline{r}) \qquad (1.17)$$

By performing some easy gaussian integration we get

$$c_n = (-1)^{n_1 n_2}\, e^{-\underline{R}_n{}^2/4} \qquad (1.18)$$

To discuss the behaviour of this overlap for very high magnetic fields it is better not to put our constants to one from the very beginning. In this way we would obtain the following wave function

$$\Psi_n(x,y) = (-1)^{n_1 n_2}(2\pi l^2)^{-1/2}\exp[- \frac{1}{4l^2} [(\underline{r}-\underline{R}_n)^2-2i(xY_n-yX_n)]] \qquad (1.19)$$

with $l^2=(eB)^{-1}$ and the overlap would be of the form

$$c_n \approx e^{-\underline{R}_n^2/l^2}$$

Therefore we see that for B going to infinity, that is for l going to zero, the overlap between the various eigenstates is one if $\underline{R}_n$ is zero (so that the two wave functions are localized both around the origin). On the contrary it goes to zero if $\underline{R}_n$ is different from zero, that is, if the functions we are considering are localized in different lattice sites. This consideration is a first indication that, in fact, the infinite magnetic field limit of a 2DEG is a classical WC. More explicitly, we mean that the wave functions describing the electrons localized around certain sites shrink to extremely picked functions whose localization characteristics resemble very much the ones of the delta functions.

At the same conclusions one can arrive if, instead of the magnetic field, the ν parameter is considered. We want to discuss briefly this point that will be considered more accurately in the next Chapter. The natural way to take into account different electron densities is to change the lattice spacing a, keeping fixed the number of electrons in the sample. This operation is allowed since the T operators still commute if (1.11) is replaced by the more general condition

$$(\underline{a}_1 \wedge \underline{a}_2)_z = 2\pi N \qquad (1.20)$$

N being an integer. Since we are considering triangular lattices with $|\underline{a}_1| = |\underline{a}_2| = a$, and since a enters in the exponent of the c_n above through the definition of the lattice sites

$$\underline{R}_n^2 = a^2(n_1^2 + n_2^2 + n_1 n_2) \qquad (1.21)$$

it is easy to deduce that, the smaller the density is, the greater is the lattice spacing a so that, from (1.18), for v going to zero, the overlap between wave functions localized in different lattice sites again tends to zero. This observation suggests an equivalence between the approach in which $B \rightarrow \infty$ and the one in which $v \rightarrow 0$ and the electron number is keepen fixed.

Another point that it is useful to stress in advance, but that will be again considered in Chapter 3, is the localization of the wave function in our problem. We see that the $\Psi_n(x,y)$ introduced before are exponentially localized. Moreover we know from (1.17) that they are not orthogonal. These two points are not unrelated. As it is in fact widely discussed in reference [24] making use of the kq-representation it is impossible to find a set of wave functions for a 2DEG at $v = 1$ that are both orthogonal and exponentially localized in one direction. This result will be restated in Chapter 3 using continuity arguments in a very different way from the one given in [24], which we consider much more satisfying. Since we can think to built up the WC constructing a lattice with the minimum spacing a obtained from (1.11), that is with

$$a = \sqrt{\frac{4\pi}{\sqrt{3}}} \tag{1.22}$$

and then to occupy each lattice site with an electron described by the function Ψ_n, then, by a quite abstract argument, the various Ψ_n cannot be orthogonal each other being exponentially localized .

We end this Chapter with the above last consideration. In the next ones many of the points already sketched will be considered again in all details and their consequences will be investigated.

In the previous Chapter we gave the form of a wave function that essentially coincides with the one proposed in [7] and therefore it is also virtually equivalent to the CDW proposed by Yoshioka et al. Here we will consider some mathematical refinements that, in our opinion, are worthwhile to discuss to better understand some points of the 2DEG that are still unclear or, at least, not well established.

We begin by building up an orthogonalized wave function starting with the one in (1.14). From this operation will appear clearly the reason why the situation with filling equal to one does not fit in our approach (However the electron-hole symmetry solves this problem!). We therefore fix ν to be 1/3 and work in this hypothesis. We use a perturbative expansion quite different from the one used in reference [7]. In particular we will show that the two approaches are numerically equivalent in a first approximation. However we go further computing explicitly the correction to the ground state energy and showing the perturbative nature of our expansion in contrast with the one proposed by Maki & Zotos. We conclude that the extremely small cusps proposed in [7] are, at least, quite improbable. We will then extend our computation to general ν and we consider in particular the limit for small ν. We confront our results with the ones obtained by Laughlin and by the CDW approach and we show that these results modify a bit the conclusions obtained in reference [21].

2.1: Orthogonal wave functions (I)

We recall that the wave function obtained by acting with the operators T on the m=0 function of the LLL has the form in (1.14)

$$\Psi_{n,m}(x,y) = (-1)^{nm} \, e^{i/2(Y_{n,m}x - X_{n,m}y)} \, \Psi_{0,0}(\underline{r} - \underline{R}_{n,m})$$

where

$$\Psi_{0,0}(x,y) = (2\pi)^{-1/2}\exp[-(x^2+y^2)/4]$$

and

$$\underline{R}_{n,m} = (X_{n,m},\ Y_{n,m}) = - a\ (n+m/2\ ,\ \sqrt{3}/2\ \ m)$$

We also recall that the overlap between functions centered in different lattice points is not zero but it is only exponentially decreasing

$$c_n = (-1)^{n_1 n_2}\ e^{-\underline{R}_n^2/4}$$

Finally we remind that we are investigating first a ν =1/3 2DEG.

A portion of the triangular Wigner lattice is showed in the figure 2 below
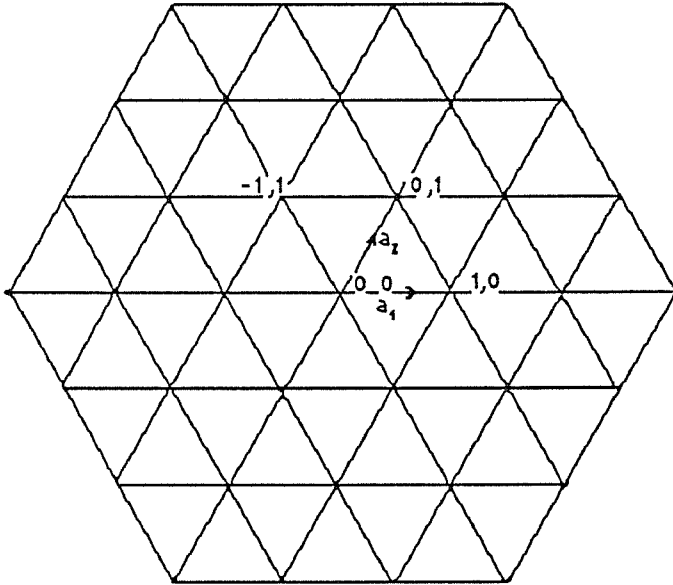
Fig. 2

where the lattice basis is also showed together with the numeration of the lattice sites. We recall that the lattice spacing in our approach is a = $|\underline{a}_1|$ = $|\underline{a}_2|$.

We can use two different approaches. In the first one, that we will call the "sub-lattice approach", the lattice spacing a satisfies condition (1.22). In this way we construct a 'minimal' lattice. In order to consider a ν =1/3 sublattice we essentially use the same idea discussed in reference

[12]: we occupy only the sites of a sublattice defined by the following vector basis

$$\underline{b}_1 = \underline{a}_1 + \underline{a}_2$$

$$\underline{b}_2 = -\underline{a}_1 + 2\,\underline{a}_2$$

It is immediate to understand that if all the sites of our minimal lattice belonging to the sublattice so defined are occupied then the filling of the 2DEG is exactly 1/3.

Alternatively we can use condition (1.20) for N=3. In this way we get a non-minimal lattice with lattice spacing $b = a\sqrt{3}$ that again corresponds to the same filling as before. This approach will be called the "non-minimal" one.

It is useful to stress that these two approaches are not totally equivalent; one can see, in fact, that in the first one the accessible fillings are $v = 1/3$, 2/3, 1/4, 3/4, 1/7, 6/7,....., so that $v = 1/5$ appears not to fit into this strategy. In the second one, on the contrary, all the $v = 1/n$ and $v = 1-1/n$ can be obtained. Therefore it appears to be a more flexible technique to deal with the 2DEG. However the sublattice approach has a certain relevance since it shows clearly the interplay between the Hilbert spaces we are considering. We mean that the Hilbert space for $v = 1/3$, $\mathcal{H}_{v=1/3}$, appears manifestly to be a subspace of $\mathcal{H}_{v=1}$, since it is constructed considering only a subset of the whole set $\{T_1^n, T_2^m \ \forall \ n,m\}$ used to built up the minimal lattice. This consideration has a certain relevance and it will be used in Chapter 4 to construct a new trial wave function for the ground state of a 2DEG.

Finally we observe also that, for what concerns computer implementation, the idea of a variable lattice spacing is much more manageable than an approach in which we have to extract the correct sublattice from the minimal one. This is, in fact, a filling dependent operation not easy to implement.

We can now start discussing the orthogonalization of the wave function and the range of v for which this operation is allowed. First we notice that a translationally invariant procedure is required in order not to break down the original invariance of the system. Therefore a Graham-Schimdt method cannot be the correct one since it necessarily refers to a

favourite site, naturally breaking in this way the translation invariance of the lattice.

We define new functions $\Omega_{n,m}(\underline{r})$ starting from the $\Psi_{n,m}$ using the following infinite sum

$$\Omega_n(\underline{r}) = \sum_i f_i \, \Psi_{n+i}(\underline{r}) \tag{2.1}$$

where again the single index notation has been used. Here the coefficients f_i must be computed requiring the orthogonality condition (2.2) below and the sum is extended to all the lattice site if we use the non-minimal approach described above or only to the sites related to the Hilbert space $\mathcal{H}_{v=1/3}$ in the sub-lattice one. Of course these functions Ω are still in the first Landau level being linear combinations of functions all belonging to the LLL.

We require Ω_n to be orthogonal each other, that is

$$(\Omega_o, \Omega_n) \approx \delta_{n,o} \tag{2.2}$$

where the $\approx$ sign must be interpreted as an approximate identity since, as we will clarify below, we use a perturbative approach.

The definition in (2.1) still maintains the required translations invariance of the system in the sense that

$$T_1^{\alpha} \, T_2^{\beta} \, \Omega_{n,m} = T_1^{\alpha} \, T_2^{\beta} \sum_{ij} f_{ij} \Psi_{i+n \, j+m} = \sum_{ij} f_{ij} \, [T_1^{\alpha} T_2^{\beta} \Psi_{i+n \, j+m}] =$$

$$= \sum_{ij} f_{ij} \Psi_{i+n+\alpha \, j+m+\beta} = \Omega_{n+\alpha,m+\beta} \tag{2.3}$$

where we have used definition (2.1) and (1.13). So the T operators are also the translation operators for the new orthogonal functions $\Omega_{n,m}$.

2.2: Computation of the expansion coefficients

Now we want to consider the consequences of the condition (2.2) on the coefficients f_{ij}. Moreover we are going to explain the meaning of such condition with particular attention to the approximate identity we have

used in that formula. To make all the steps more explicit we use again the double index notation.

Using the unitarity of the operators T, the definition (1.17) of the coefficients c_n and formulas (2.1) and (2.2) we have

$$\delta_{n,o}\delta_{m,o} = \sum_{ijls} f_{ij}* f_{ls} (\Psi_{i,j},\Psi_{n+l,m+s}) =$$

$$= \sum_{ijls} f_{ij}* f_{ls} (\Psi_{o,o},\Psi_{n+l-i\ m+s-j}) = \sum_{ijls} f_{ij}* f_{ls} c_{n+l-i\ m+s-j}$$

We remind that the above steps are not correct if the wave function introduced in [7] is used, as we have already discussed in Chapter 1. We define the discrete Fourier transform by the

$$F(k,q) \equiv \sum_{nm} f_{nm} e^{ikna+iqma} \tag{2.4}$$

$$f_{nm} = \left\{\frac{a^2}{2\pi}\right\} \int_0^{2\pi/a} dk \int_0^{2\pi/a} dq\ e^{-ikna-iqma} F(k,q) \tag{2.5}$$

with k and q ranging between 0 and $2\pi/a$. Using these definitions the above equation can be rewritten, after multiplying both side for the factor $e^{ikna+iqma}$ and summing over n and m, in the form

$$|F(-k,-q)|^2\ C(k,q) = 1$$

$C(k,q)$ being the Fourier transform of the coefficients c_n. From the explicit expression (1.18) we can see that $c_n = c_{-n}$. Therefore one easily obtains that $C(k,q) = C(-k,-q)$. We conclude that the above equation can be conveniently put in the form

$$|F(k,q)|^2\ C(k,q) = 1 \tag{2.6}$$

which of course is solved by

$$F(k,q) = \frac{e^{i\Phi(k,q)}}{\sqrt{C(k,q)}}$$

where the function Φ is any real function of the variables k and q. Throughout this work we will choose Φ to be zero so that the final result is

$$F(k,q) = \frac{1}{\sqrt{C(k,q)}} \qquad (2.7)$$

In order to obtain the coefficients of the sum (2.1) we therefore need to first know the function C(k,q) and then to transform back the result of (2.7). Using the definition (2.4) we define

$$C(k,q) \equiv \sum_n c_n \, e^{ikn_1a + iqn_2a} \qquad (2.8)$$

which we write as

$$C(k,q) = 1 + \sum_{n \neq 0} c_n \, e^{ikn_1a + iqn_2a} \qquad (2.9)$$

where the first term is of course the value that the above sum gets for n=0. Such a separation of contributions, which is always allowed, turns out to have a practical utility for the analysis of the convergence of the series in (2.1) only for $v \leq 1/3$. In fact if we compute the overlap coefficients $c_{1,0}$ between functions centered in adjacent sites of the non-minimal lattice we see that $|c_{1,0}|$ is equal to 0.1630 for $v = 1$, to 0.0043 already for $v = 1/3$, and decreases more and more for smaller v. Since each lattice site has six neighbourhood sites we see that, defining a function g(k,q) via the

$$g(k,q) \equiv \sum_{n \neq 0} c_n \, e^{ikn_1a + iqn_2a} \qquad (2.10)$$

this function can in principle be of order one for $v = 1$ while we claim that it is much less that one for filling $v \leq 1/3$. We will prove this assertion below in many details.

In order to discuss the convergence of the series in (2.1) we use an analyticity argument for the function F(k,q). It is well known that the

coefficients of the Fourier transform of an analytic function of period $2\pi/a$ (such function is continuous and periodic together with all its derivatives) decrease faster than any power of $1/k$ with increasing k, [25]. Therefore we want to discuss the analyticity property of $F(k,q)$. First of all it is easy to estimate that for $v \leq 1/3$ the function $g(k,q)$ cannot be of order one for k and q ranging between 0 and $2\pi/a$. We can sketch this result is the following way. First of all we have

$$| g(k,q)| \leq \sum_{n \neq 0} |c_n| = \sum_{n \neq 0} e^{-R_n^2/4} =$$

$$= \sum_{n \neq 0} \exp \left\{ -\pi \sqrt{3} (n_1^2 + n_2^2 + n_1 n_2) \right\}$$

where we have used the lattice for $v = 1/3$ and with lattice spacing $b = a\sqrt{3}$. This sum can be estimated in a simple way by counting, in figure 2, the number of lattice sites that contribute to the sum defining $g(k,q)$ for each 'lattice shell', that is, for each set of lattice points that have the same distance from the origin of the crystal. Calling $\lambda = e^{-\pi\sqrt{3}}$ we get

$$| g(k,q)| \leq 6\lambda + 12\lambda^4 + 18\lambda^9 + ... = 6\sum_{k=1}^{\infty} k\lambda^{k^2}$$

which has been numerically estimated to be, up to the fourth significative digit, equal to 6λ. For obtaining an analytical estimate it is possible to add positive contributions in such a way to dominate $| g(k,q)|$ with the following expression

$$| g(k,q)| \leq 6\lambda + 12\lambda^2 + 18\lambda^3 + ... = 6 \sum_{k=1}^{\infty} k\lambda^k \leq 6 \frac{\lambda}{(1-\lambda)^2} \approx 0.0258$$

This is obviously an overestimate that is, however, sufficient to show that the result is still much less than 1, proving in this way our original claim.

An analogous result can also be proven if in (2.10) we consider k and q as complex quantities, $k = k_R + i\ k_I$ and $q = q_R + i\ q_I$. One can conclude that it exists a strip of the real axis k and q, $k_R \in (0, 2\pi/a)$, $q_R \in (0, 2\pi/a)$, $k_I \in$ (-

v, v) and $q_I \in (-v, v)$, v being estimated to be of the order $\pi/2a\sqrt{3}$, in which $C(k,q)$ cannot be equal to zero. From (2.7) this implies that $F(k,q)$ does not have any singularity in this strip so that its Fourier anti-transform has remarkable decay properties. We will see explicitly that, in fact, the f_{ij} coefficients of the (2.1) exponentially go to zero. Making use of (2.7), and (2.9) we can expand $F(k,q)$ in the form

$$F(k,q) \approx 1 - \frac{1}{2} \sum_{j \neq 0} c_j\, e^{ikj_1a+iqj_2a} + \frac{3}{8} \sum_{j\,s \neq 0} c_j c_s\, e^{ik(j_1+s_1)a+iq(j_2+s_2)a} \quad (2.11)$$

which, once it is inserted in (2.5), gives the following result for the expansion coefficients:

$$f_n \approx \delta_{n,o} - \frac{1}{2} c_n + \frac{3}{8} \sum_{s \neq 0}^{(s \neq n)} c_{n-s}\, c_s \quad (2.12)$$

We have used above the $\approx$ symbol since we are performing a perturbation expansion whose validity will be supported by some estimate about the contributions we are neglecting. The possibility of performing the perturbative expansion in (2.12) is, of course, strongly related to the values the coefficients c_s take for the various values of the filling. We have already showed that for $v = 1/3$ we have $|c_{1,0}| = 0.0043$ and that $|c_{2,0}| \ll |c_{1,0}|$ so that an expansion as the one above seems to be reasonable. Of course things go better if $v < 1/3$ since the coefficients c_s are even smaller. For $v \approx 1$, on the contrary, the overlap is so high that we cannot hope to perform any perturbative expansion of the kind we have just introduced. This problem can be solved by the electron-hole symmetry of the Hamiltonian H, see, for example, reference [13]. This consists in the invariance, but for some constants, of H under the transformations $b_i = c_i^*$ and $b_i^* = c_i$, b_i^* and c_i^* being respectively the creator operators for the electrons and the holes. To be explicit the above transformation leads to $H(c_i,v) = H(b_i,1-v)$ up to a c-number. This property allows us to deal with an electron filling near to one as if we were dealing with a $v \approx 0$ hole lattice so that our method can be translated in the hole language and it can still be applied.

2.3: Orthogonal wave functions (II)

We now substitute the form of the coefficients given by (2.12) in the formula (2.1), obtaining the following expression of the orthogonalized wave functions

$$\Omega_i \approx \Psi_i - \frac{1}{2} \sum_{n \neq 0} c_n \Psi_{i+n} + \frac{3}{8} \sum_n \sum_{s \neq 0}^{(s \neq n)} c_{n-s} c_s \Psi_{i+n} \qquad (2.13)$$

The utility of this formula, in this Chapter, is that it gives the possibility of performing a perturbative expansion of the ground state energy. We will use as expansion parameter the coefficient $c_{1,0} \approx \exp\{-\underline{R}_{1,0}^2/4\}$, where $|\underline{R}_{1,0}|$ is the distance between the first (occupied) site and the origin. We use here the non-minimal lattice notation. Obviously a first control on the validity of the expansion (2.13) is obtained from the computation of $c_{1,0}$ for each value of the filling. This gives a sort of upper bound for the value of the filling for which expansion (2.13) is meaningful since, as we have already noticed, $|c_{1,0}(v)|$ is an increasing function of v.

It is possible to compute the scalar product between two orthogonalized functions and therefore to verify the validity of condition (2.2). We have

$$(\Omega_o, \Omega_n) = \delta_{n,o} + O(c_{1,0}^3) \qquad (2.14)$$

which shows that the Ω_i wave functions are orthonormal up to corrections of the $c_{1,0}^3$ order. Since for filling 1/3 $c_{1,0}^3 \approx 8 \cdot 10^{-8}$, one gets the feeling that our perturbative expansion is meaningful.

From now on we will use the equal sign instead of the $\approx$ often used previously neglecting in this way the $O(c_{1,0}^3)$ corrections. However their effect will be estimated at the end of the Chapter to verify the validity of our approach.

We now use equation (2.13) in order to discuss the localization of the wave function. We see that, up to the desired order, the function Ω_i appears to be essentially exponentially localized around the lattice site $i = (i_1, i_2)$ with small corrections of the order $c_{1,0}$, also exponentially decaying, coming from the first shell around this site and very small contributions, $O(c_{1,0}^2)$, from the site i itself, and from the two surrounding shells. Therefore we have an almost exponential localization together with

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orthogonality. We have already anticipated the fact that, for $v = 1$, orthogonality requires a very slower electron wave function localization at least in one space direction: this is reflected in our procedure by the fact that, as already discussed, a perturbative expansion as the one in (2.13) is meaningless due to the non sufficiently small value of the coefficients c_n corresponding to such a filling. In particular, for example, condition (2.14) does not imply any more orthogonality of the wave functions since the $O(c_{1,0}^3)$ corrections can be of order one. This means that in (2.13) we are not allowed to restrict the summation to the second order in c_n since the rest we should neglect gives a contribution relevant for the correct definition of the orthogonalized wave function.

The next step consists in constructing the N-electrons wave function. We restrict to a single Slater determinant, that is, we do not consider correlations between electrons, and assume an ansatz 'ground' state given by the following anti-symmetrized function

$$\Lambda_0(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Omega_1(1) & \Omega_2(1) & \ldots & \Omega_N(1) \\ \Omega_1(2) & \Omega_2(2) & \ldots & \Omega_N(2) \\ \ldots & \ldots & \ldots & \ldots \\ \Omega_1(N) & \Omega_2(N) & \ldots & \Omega_N(N) \end{vmatrix} \quad (2.15)$$

where we have used an obvious notation. Λ_0 is normalized up to the $c_{1,0}^3$ order due to the (2.14). We have, in fact

$$< \Lambda_0, \Lambda_0 > = 1$$

We recall the original perturbative meaning of the equal sign in the equality above.

Λ_0 is the wave function whose energy we are now going to compute in the next Section.

2.4: Ground state energy

First of all we recall that, being Λ_0 normalized, the energy of such a state is

$$E(N) = < \Lambda_0, H \Lambda_0 >$$

H being the Coulomb interaction between electrons

$$H = \frac{1}{2} \sum_{i \neq j} \frac{1}{|\underline{r}_i - \underline{r}_j|}$$

and where we still have not considered the subtraction of the positive background energy.

Here we neglect the kinetic term that is a constant when the electrons are in the LLL, as it happens for strong magnetic fields.

For a system of N electrons we obtain, in the Hartee-Fock approximation, the following expression:

$$E(N) = \frac{1}{2} \sum_{i \neq j}^{N} [E_d(i,j) - E_s(i,j)] \tag{2.16}$$

where

$$E_d(i,j) = \int d^2\underline{r}_1 \, d^2\underline{r}_2 \, \frac{|\Omega_i(\underline{r}_1)|^2 \, |\Omega_j(\underline{r}_2)|^2}{|\underline{r}_1 - \underline{r}_2|} \tag{2.17}$$

and

$$E_s(i,j) = \int d^2\underline{r}_1 \, d^2\underline{r}_2 \, \frac{\Omega_i^*(\underline{r}_1) \, \Omega_j^*(\underline{r}_2) \, \Omega_j(\underline{r}_1) \, \Omega_i(\underline{r}_2)}{|\underline{r}_1 - \underline{r}_2|} \tag{2.18}$$

In order to subtract the positive background we use the result of reference [6]. Here the energy of a classical system of electrons, represented by delta functions centered in the various lattice sites, is computed after subtracting the interaction of the electrons with a positive uniform background. Let us introduce now the interaction energy $E_b(N)$ among the N electrons and the background and let $E_w(N)$ be the energy of the classical WC without eliminating the background. In this way we can compute the mean (subtracted) energy for particle in the following way:

$$E_0 = \lim_{N \to \infty} \frac{E(N) - E_b(N)}{N} =$$

$$= \lim_{N \to \infty} \left\{ \frac{E(N) - E_w(N)}{N} + \frac{E_w(N) - E_b(N)}{N} \right\} \qquad (2.19)$$

Here, of course, the second contribution is the classical Wigner energy with the background subtraction, see [6]; the first piece is instead the term we are computing in (2.16) minus the classical contribution coming from the interaction between the electrons in the WC. We call

$$E_w = \lim_{N \to \infty} \left\{ \frac{E_w(N) - E_b(N)}{N} \right\} \qquad (2.20)$$

and

$$\delta E = \lim_{N \to \infty} \left\{ \frac{E(N) - E_w(N)}{N} \right\} \qquad (2.21)$$

Obviously E_w is known from [6] while the correction δE is what we need to compute. We recall again that we are assuming for the time being a filling equal to $1/3$. We will generalize to an arbitrary v later on.

We add few words to notice that we need to consider a periodic positive background in order to simplify the computation. In fact for a system of electrons and, say, ions, in a complete energetic computation one must consider three contributions: E_{ee}, E_{ei} and E_{ii}, which are, respectively, the electron-electron, the electron-ion and the ion-ion energies. One can show that if the ions are periodically disposed in the lattice then the sum of E_{ei} and E_{ii} is equal to $E_{ei}/2$. This allows one to consider simply the interaction between electrons and ions in order to subtract the positive background.

In order to compute $E(N)/N$ we fix the position of the j-th electron to be, for instance, $j=(0,0)$. We have:

$$E_I = \lim_{N \to \infty} E(N)/N = \frac{1}{2} \sum_{i \neq 0} \left\{ E_d(i,0) - E_s(i,0) \right\} \qquad (2.22)$$

where the $E_d(i,0)$ and $E_s(i,0)$ are defined above.

We defer to Appendix 2 and Appendix 3 for all the technical details. In the first one we compute the generic matrix element of the Coulomb potential between the wave functions Ψ_n and we analyze its expansion for large values of the argument; in the second one we give the explicit form of δE. Here we only sketch the main steps and the results without giving all the details.

In computing E_I we must substitute (2.13) in the integrals defining E_d and E_s. Therefore the summation in (2.22) contains many contributions some of which, the ones of order greater than $c_{1,0}^2$, will be neglected in the computation, see Appendix 3. This approximation is justified in Appendix 2, where we briefly discuss the characteristic of the integrals defining the matrix elements of modifying the behaviour of the various contributions in a "safe way". To be more explicit a term, for instance, of the form $c_{1,0}^3 V_{ijkl}$ cannot give, for some peculiar value of the indexes i,j,k,l, a net contribution of the order $c_{1,0}^2$. This property is crucial to build up a well-defined perturbative expansion in which all the contributions can be safely and easily controlled, characteristic that, in our opinion, is totally absent in the approach discussed in [7]. We have already pointed out that, in this reference, no estimate a priori can be easily made on the contributions coming from the various expansion terms. Therefore we must explicitly computate these contributions before neglecting in order to explicitate their effective weight in the expansion.

Our perturbative scheme, as it has already been anticipated, consists in considering only the contributions coming from terms whose *net* order is less or equal to $\exp\{-\underline{R}_{10}^2/4\}^2$, neglecting all the successive power of the above exponent. We define "*net* order" of a term the power of $\exp\{-\underline{R}_{10}^2/4\}$ obtained both from the exponential dependence of the matrix elements and from the coefficients c_n. Of course this scheme seems to be justified already for filling $\nu \leq 1/3$, since for such a filling the exponent above is very small as we have already discussed in Section 2.2.

Once the perturbative approach has been discussed we can start sketching the explicit computation of the ground state energy. The general matrix element has the following form

$$V_{ijkl} = \int \frac{d^2\underline{r_1}\, d^2\underline{r_2}}{|\underline{r_1} - \underline{r_2}|}\, \Psi_i{}^*(\underline{r_1})\, \Psi_j(\underline{r_1})\, \Psi_k{}^*(\underline{r_2})\, \Psi_l(\underline{r_2}) \qquad (2.23)$$

which is exactly computed in Appendix 2 for any values of the indexes. Here we report only the final result for reader's convenience. We define the following quantities

$$q_1 = \frac{1}{2}(\underline{R_i} + \underline{R_j}); \quad q_2 = \frac{1}{2}(\underline{R_k} + \underline{R_l}); \quad \underline{R}_o = q_1 - q_2$$

$$\underline{\Delta}_1 = \underline{R_j} - \underline{R_i}; \quad \underline{\Delta}_2 = \underline{R_l} - \underline{R_k}; \quad \underline{\Theta}_1 = (\Delta_{1y}, -\Delta_{1x}); \quad \underline{\Theta}_2 = (\Delta_{2y}, -\Delta_{2x})$$

$$(2.24)$$

$$A_1 = \frac{1}{2}(\underline{R_i} - \underline{R_j})^2; \quad A_2 = \frac{1}{2}(\underline{R_l} - \underline{R_k})^2; \quad \underline{v} = \underline{\Theta}_1 - \underline{\Theta}_2; \quad \underline{v_c} = \frac{1}{2}\underline{v} - i\,\underline{R}_o$$

$$\Phi_1 = \exp\left\{\frac{i}{2}(q_1\cdot\underline{\Theta}_1 + q_2\cdot\underline{\Theta}_2)\right\}$$

so that the result can be written as

$$V_{ijkl} = (-1)^{i_1 i_2 + j_1 j_2 + k_1 k_2 + l_1 l_2}\, \Phi_1 \sqrt{\frac{\pi}{4}}\, e^{-(A_1+A_2)/2}\, e^{\underline{v_c}^2/8}\, I_0(\underline{v_c}^2/8) \qquad (2.25)$$

I_0 being the modified Bessel function of the first order. We notice that our result reproduces the ones of [7] when specialized to the situations with i=j, k=l and i=l, j=k.

Using the asymptotic expansion of I_0 as it is given in many standard books, see for example [26], one can obtain the behaviour of the matrix elements above for large values of $\underline{v_c}^2/8$. This behaviour will be explicitly obtained in Appendix 2. We report the result below and we see that such an asymptotic behaviour contains an exponential dependence on the lattice vectors $\underline{R}_n$, n=i,j,k,l. Since in our approach only the terms up to the $(\exp\{-\underline{R}_{10}^2/4\})^2$ order must be considered not all the original c_{10}^2 contributions will play some rôle; in fact it may happen that some of the matrix elements V_{ijkl} give an extra exponential decreasing factor, for instance another $\exp\{-\underline{R}_{10}^2/4\}$, so that the net contribution turns out to be negligible in our scheme.

What is out of doubt, and it is discussed in some details in Appendix 2, is that for no value of the indexes the matrix element V_{ijkl} can **increase** the net order of a term. This is a crucial feature of our approach since otherwise all our efforts of getting an a priori control of the various contributions of the perturbative expansion would be vain.

We report here the results of Appendix 2, where the following asymptotic behaviour is deduced:

- for $Re[\underline{v}_c^2] > 0$

$$V_{ijkl} \sim \exp\left\{-\frac{1}{4}[2(A_1-A_2) - Re[\underline{v}_c^2]]\right\}$$

- for $Re[\underline{v}_c^2] \leq 0$

$$V_{ijkl} \sim \exp\left\{-\frac{1}{2}(A_1-A_2)\right\}$$

where A_1 and A_2 are defined in (2.24). In Appendix 2 it is also discussed an upper bound for the asymptotic behaviour of V_{ijkl}, useful in order to get rid of the terms with $Re[\underline{v}_c^2]$ that are not simple to be read nor useful in many relevant estimates.

Before giving the numerical result we recall that $\lim_{N\to\infty} E_w(N)/N$ must be subtracted to E_I that, otherwise, would turn out to be divergent in the limit of N going to infinity. It is simple to compute this divergent contribution: we simply observe that a classical WC is one in which all the electrons are exactly localized in single points so that they are described by delta functions centered in the various lattice sites. Therefore, we deduce that the contribution of such a crystal is exactly what one expect from a classical one:

$$\lim_{N\to\infty} \frac{E_w(N)}{N} = \frac{1}{2}\sum_{i\neq 0} \frac{1}{|R_i|} \tag{2.26}$$

Taking into account all these considerations, we can use a computer routine to compute the sum over the lattice sites of the various contributions to δE. The summation is extended to a lattice big enough to ensure that the contributions we neglect do not really modify the result of

the finite summation. This means that we consider lattices so big that the contribution coming from the extra lattice sites is extremely small. To be concrete we consider, for a 1/3 filling, a 1200 x 1200 lattice. Of course, being the summation convergent, we do not need to extend the sum to a sublattice of the whole Z^2 that has the same exagonal symmetry of the original cells. Moreover, due to the exponentially decreasing factors appearing in the various contributions to δE, for $v < 1/3$ we can use smaller lattices since the convergence is certainly faster.

We now want to give some numbers that we believe are relevant for understanding the rôle of the corrections coming from the essential non-ortogonality of the wave functions. In this way we control the effects that are only estimated in [7]. We write δE in (2.21) in a more extended and useful form. We put

$$\delta E = E_d + \delta E_d - E_s - \delta E_s \tag{2.27}$$

Here E_d and E_s are the direct and the exchange contributions with the subtraction already considered, δE_d is the correction to the direct term of the energy due to the overlap between the eigenfunctions Ψ and δE_s is the analogous term for the exchange contribution. This is the reason why we call δE_d and δE_s "non-orthogonality contributions". The explicit form of these terms can be deduced from Appendix 3. Here we remind only the exact form of E_d and of E_s. We have:

$$E_d = \frac{1}{2}\sqrt{\frac{\pi}{4}}\sum_{i\neq 0} e^{-R_i^2/8}\, I_0(R_i^2/8) - \frac{1}{2}\sum_{i\neq 0}\frac{1}{|R_i|} \tag{2.28}$$

and

$$E_s = \frac{1}{2}\sqrt{\frac{\pi}{4}}\sum_{i\neq 0} e^{-3\,R_i^2/8}\, I_0(R_i^2/8) \tag{2.29}$$

For $v = 1/3$ we obtain the following numbers:

$E_d = 0.0656$ $E_s = 0.0030$ $\delta E_d = 0.0001$ $\delta E_s = 0$

We know, for example from reference [22], that the classical Wigner energy in (2.20) is, for the present value of v, $E_w = -0.4515$. Therefore the ground state energy E_0 is, see (2.19),

$$E_0 = E_w + \delta E = -0.3888 \tag{2.30}$$

which is essentially identical to the one of [7], [8] and [11]. The minimal difference is due to the δE_d contribution that in [7] is not taken into account and that slightly raises the result.

To end this Section we discuss a further estimate that has been conducted. We have considered the terms of the order $c_{1,0}^3$ and we have evaluated the corrections arising from such contributions. It is useful to remind here only the fact that, to take correctly into account these corrections, we have to modify the form of the wave function Ω_n in (2.13) adding one more term:

$$\Omega_i \approx \Psi_i - \frac{1}{2} \sum_{n \neq 0} c_n \Psi_{i+n} + \frac{3}{8} \sum_n \sum_{s \neq 0}^{(s \neq n)} c_{n-s} c_s \Psi_{i+n} +$$

$$- \frac{5}{16} \sum_n \sum_{m \neq 0 \; l \neq 0}^{(m+n \neq l)} c_{n+m-l} c_m c_l \Psi_{i+n}$$

since the last term contributes to the relevant order for m, l, $n+m-l$ all in the first shell. Moreover, since $c_{1,0}^3 = c_{3,0}$, also the term linear in the c_n gives a contribution to this order. Overestimating the integrals with the worst possible behaviour compatible with the absence of further divergence at this order, that is with $1/|R_i|^3$, we see that the correction to the ground state energy E_0 coming from these terms is less than $4 \cdot 10^{-6}$, so that it can securely be neglected.

We conclude noticing that a full control of all the contributions is allowed by our approach: this is in our opinion the main advantage with respect to the ideas discussed in [7] where this control does not exist, or, at least, is not as direct as for our strategy.

2.5: Other fillings

We now sketch the computation of the ground state energy for fillings smaller than 1/3. The idea is that different ν are related to different lattice constant a, a being determinated by the condition (1.20)

$$(\underline{a}_1 \wedge \underline{a}_2)_z = 2\pi \, N$$

with $a = |\underline{a}_1| = |\underline{a}_2|$. Since the i-th lattice site is described by the vector $\underline{R}_i$ whose modulus square has the expression

$$\underline{R}_i^2 = a^2 (i_1^2 + i_2^2 + i_1 \, i_2)$$

and since the minimal a^2 (obtained for N=1) is $4\pi/\sqrt{3}$ we can define, for a generic $\nu = 1/N$, a new non-minimal lattice for which the vectors $\underline{R}_i$ satisfy the condition:

$$\underline{R}_i^2 = \frac{1}{\nu} \frac{4\pi}{\sqrt{3}} (i_1^2 + i_2^2 + i_1 \, i_2) \tag{2.31}$$

We have used (2.31) to compute the various contributions to δE in (2.27). From (2.28), (2.29) and (2.31) it appears quite clear the way in which the filling appears in E_d and E_s: essentially we must substitute the minimal lattice constant whose square is $4\pi/\sqrt{3}$ with the lattice constant related to the particular ν we are considering: $\sqrt{4\pi/(\nu\sqrt{3})}$. The same consideration applies also to δE_d and δE_s, which, however, are so small that can be both neglected already for $\nu = 1/5$. We have:

- for $\nu = 1/5$

$$E_d = 0.0276 \qquad E_s = 0.0001 \qquad \delta E_d = 0 \qquad \delta E_s = 0$$

$$E_w = -0.3497$$

and therefore

$$E_0(1/5) = -0.3222 \tag{2.32}$$

- for $\nu = 1/7$

$$E_d = 0.0161 \qquad E_s = 0 \qquad \delta E_d = 0 \qquad \delta E_s = 0$$

$$E_w = -0.2956$$

and therefore

$$E_0(1/7) = -0.2795 \qquad\qquad (2.33)$$

- for $\nu = 1/9$

$$E_d = 0.0107 \qquad E_s = 0 \qquad \delta E_d = 0 \qquad \delta E_s = 0$$

$$E_w = -0.2607$$

and therefore

$$E_0(1/9) = -0.2500 \qquad\qquad (2.34)$$

We observe that the non orthogonality corrections, which as we have already discussed are the contributions δE_d and δE_s, are really very small, even for a filling 1/3. So, from a numerical point of view, the Maki and Zotos' approach is justifiable. Furthermore, for $\nu \leq 1/7$, the same exchange contribution vanishes up to the relevant approximation, so that the classical nature of the WC begins to appear. Third, the direct contribution becomes smaller and smaller, so that it seems reasonable to expect that in the limit of very small electron fillings our model tends to a classical WC. We analyze the analyticity of the function $E_0(\nu)$ in the next Section.

2.6: Other approaches: a parallel

We are now going to discuss essentially two points: a comparison of the above energy values with the ones obtained by other approaches, and the limit of such approaches for $\nu \rightarrow 0$. We indicate with $E^{CDW}(\nu)$, $E^L(\nu)$ and $E^{TP}(\nu)$ respectively the energy obtained using the CDW approach, the Laughlin's wave function and the scheme proposed by Tosatti and

Parrinello. Some of the values are obtained using the interpolation formulas given by Levesque et al. in [21]:

$$E^L(\nu) = -0.7821 \sqrt{\nu} \ (1- 0.211 \ \nu^{0.74} + 0.012 \ \nu^{1.7}) \qquad (2.35)$$

$$E^{CDW}(\nu) = -0.7821 \sqrt{\nu} \ (1- 0.372 \ \nu - 0.013 \ \nu^2) \qquad (2.36)$$

where (2.35) is valid for any ν between 0 and 1, while (2.36) holds for ν less than 1/5. This is slightly in contrast with what it is claimed in [21] where the $E^{CDW}(\nu)$ is assumed to work already for $\nu \le 1/3$, while an explicit confront with the values given, for instance, in [22] shows that the expression in (2.36) gives only an approximation of the 'true' results for $\nu = 1/3$ and $\nu = 1/5$. From the above formulas, from [13] and from [22] we get the following values of the energy:

$$E^{CDW}(1/3) = -0.389 \qquad E^{CDW}(1/5) = -0.322$$

$$E^{CDW}(1/7) = -0.2798 \qquad E^{CDW}(1/9) = -0.2499$$

$$E^L(1/3) = -0.410 \qquad E^L(1/5) = -0.328$$

$$E^L(1/7) = -0.2810 \qquad E^L(1/9) = -0.2500$$

$$E^{TP}(1/3) = -0.364 \qquad E^{TP}(1/7) = -0.257$$

We see immediately that the energetic values of the Magnetic Wigner commensurate superlattice discussed in [12] by Tosatti and Parrinello are too high compared to the other approaches. So it is a non variationally optimized version of the CDW approach. In Chapter 1 we have already anticipated what in our opinion is the main reason of such a behaviour: the authors in [12] start with an Hamiltonian symmetric in x and y and define eigenfunctions in which this symmetry is lost. As a consequence the energy of this asymmetric system rises.

For what concerns our values and the ones obtained by a CDW state, we see that they are essentially identical. This result agrees with the final consideration of the previous Section, where we have stated the numerical irrelevance of the orthogonality corrections to the wave functions proposed by Maki & Zotos. Finally, we see that, up to $\nu = 1/7$, Laughlin energy is

smaller than our energy while, for $v = 1/9$, they coincide. We will analyze this feature in more details below. In our opinion it seems to be therefore $1/9$ the critical value of the electron filling in correspondence of which a transition from the incompressible liquid to the crystalline phase occurs. Of course another phase transition between a liquid and a hole crystal is expected for $v = 1-1/9$.

To show that $1/9$ is the critical filling we now obtain an asymptotic expansion of our energy as a function of v for small values of the filling, analogous to the expansions given in (2.35) and (2.36).

We start claiming that, for $v \to 0$, the only relevant contributions to E_0 in (2.19), $E_0(v) = E_w(v) + \delta E(v)$, are the well known Wigner energy and the direct contribution $E_d(v)$ explicitated in (2.28). In order to prove this we consider first the exchange term in (2.29):

$$E_s = \frac{1}{2}\sqrt{\frac{\pi}{4}} \sum_{i \neq 0} e^{-3 \underline{R}_i{}^2/ 8} \, I_0(\underline{R}_i{}^2/8)$$

and we use the asymptotic expansion of the modified Bessel function I_0, see [26], which holds for positive arguments. We have, for $z \to +\infty$:

$$I_0(z) \approx \frac{e^z}{\sqrt{2\pi z}} \left\{ \frac{\Gamma(1/2)}{\Gamma(1/2)} - \frac{1}{2z} \frac{\Gamma(3/2)}{\Gamma(-1/2)} + \frac{1}{4z^2} \frac{\Gamma(5/2)}{2! \, \Gamma(-3/2)} \right\} \qquad (2.37)$$

so that, recalling that from formula (2.31) if v goes to zero then $\underline{R}_i{}^2$ goes to infinity, the exchange term can be approximated by the following expression:

$$E_s = \frac{1}{2} \sum_{i \neq 0} e^{- \underline{R}_i{}^2/ 4} \frac{1}{|\underline{R}_i|} \left\{ 1 + \frac{1}{|\underline{R}_i|^2} \right\}$$

Let us introduce now a filling independent vector $\underline{P}_i$, using once again formula (2.31). We define

$$\underline{P}_i{}^2 = \frac{4\pi}{\sqrt{3}} \left(i_1{}^2 + i_2{}^2 + i_1 \, i_2 \right) \qquad (2.38)$$

so that

$$\underline{R}_i^2 = \frac{1}{\nu} \ \underline{P}_i^2 \tag{2.39}$$

We write therefore E_s in the form

$$E_s = \frac{1}{2} \sum_{i \neq 0} e^{-\underline{P}_i^2/4\nu} \ \frac{\sqrt{\nu}}{|\underline{P}_i|} \left\{ 1 + \frac{\nu}{|\underline{P}_i|^2} \right\}$$

which goes to zero exponentially when ν approaches zero.

An analogous decay property is obtained in δE_d and δE_s since both of them, see Appendix 3, contains decreasing exponentials like the one in E_s. Actually these other exponentials are even faster in approaching zero since their arguments are in general greater than $\underline{P}_i^2/4$.

Let us now consider the direct term minus the background subtraction. If we use expansion (2.37) in such a term, E_d,

$$E_d = \frac{1}{2} \sqrt{\frac{\pi}{4}} \sum_{i \neq 0} e^{-\underline{R}_i^2/8} \ I_0(\underline{R}_i^2/8) - \frac{1}{2} \sum_{i \neq 0} \frac{1}{|R_i|}$$

we get the following result:

$$E_d = \frac{1}{2} \sum_{i \neq 0} \frac{1}{|\underline{R}_i|^3} \left\{ 1 + \frac{9}{2} \frac{1}{|\underline{R}_i|^2} \right\}$$

or, expliciting the dependence on ν:

$$E_d = \frac{\nu^{3/2}}{2} \sum_{i \neq 0} \frac{1}{|\underline{P}_i|^3} \left\{ 1 + \frac{9}{2} \frac{\nu}{|\underline{P}_i|^2} \right\}$$

Since the ν dependence in E_d is polynomial while the other contributions to the energy decays exponentially for small ν, our original claim is justified, and therefore E_d and E_w are the only contributions we need to consider to study the small ν-dependence of the ground state energy $E_0(\nu)$. Of course ν must be less than $1/3$ since we know from Section 2.4 that for this value of the filling the exchange contribution is slightly different from zero.

We now compute the numerical coefficients

$$k_1 = \frac{1}{2} \sum_{i \neq 0} \frac{1}{|\underline{P}_i|^3} \qquad\qquad k_2 = \frac{9}{4} \sum_{i \neq 0} \frac{1}{|\underline{P}_i|^5}$$

that turn out to be $k_1 = 0.2814$ and $k_2 = 0.1073$. Moreover we already know, see for instance [22], that in our unities the Wigner energy as a function of the filling has the following expression: $E_w(\nu) = -0.7821 \sqrt{\nu}$. The result is therefore that the ground state energy can be written as:

$$E_0(\nu) = -0.7821 \sqrt{\nu} \; (1 - 0.3598 \; \nu - 0.1372 \nu^2) \qquad\qquad (2.40)$$

This function looks very much the same as the $E^{CDW}(\nu)$ of (2.36), as one could expect since the approaches are very similar, at least for small values of ν. On the contrary it is quite different from the Laughlin energy $E^L(\nu)$. We will now compare (2.40) with the formulas given in (2.35) and (2.36).

Let us first observe that formula (2.40) gives the following values of the energy: $E_0(1/3) = -0.3905$, $E_0(1/5) = -0.3223$, $E_0(1/7) = -0.2796$, $E_0(1/9) = -0.2498$. All of these are almost identical to the ones explicitly obtained in Section 2.4 and 2.5. This is essentially due to the small values of the exchange term for these values of the filling. We notice that this holds true even for the only filling, $\nu = 1/3$, for which the exchange term plays a relevant rôle.

We see from this formula that, at least in the approximation we are working, $E_0(\nu)$ is analytical in ν. This is expected to be true also for ν a little bigger than 1/3 due to the fact that the only dependence on ν in the complete $E_0(\nu)$, see (2.30), is exponential and polynomial. Therefore it seems that no cusp can be obtained through this procedure. However an interesting remark must be done: in obtaining the expansion (2.40) we have implicitly assumed that continuous variations of the filling are available in our approach. As a matter of fact this is an extrapolation since for a value of ν different from 1/n and from 1-1/n we know that the operators T_j do not commute. This implies that the wave functions $\Psi_{n,m}$ are defined up to a phase path-depending. Of course this feature enriches our model giving it more freedom. Nevertheless it seems not so natural to expect that this extra phase, which is of course a function of ν, can be responsible of the cusps in $E_0(\nu)$. We remind that a possible way out is

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however given by CRE processes briefly discussed in Section 1.2, by means of which cusps in energy are obtained.

In figure 3 we compare $\Delta E_0(v) = E_0(v) - E_w(v)$ with $\Delta E^L(v) = E^L(v) - E_w(v)$ for filling values less than 1/5. We recall that the relevant range for which expansion (2.40) has been obtained is $v < 1/3$.
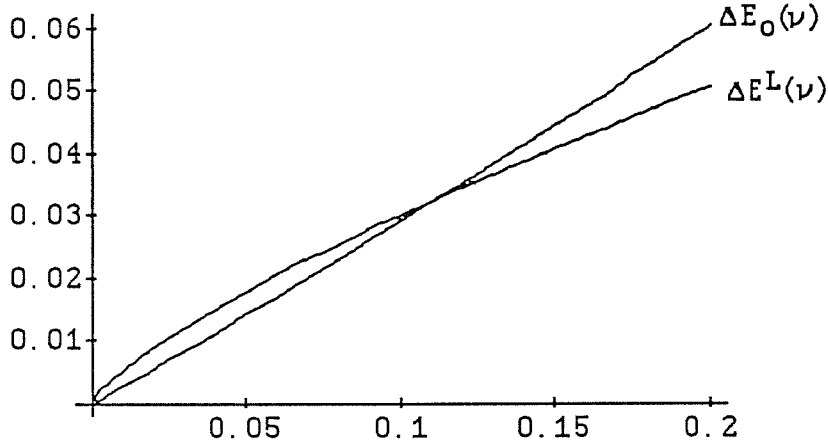

Fig. 3

From this figure we can observe that there is a full range of values of v for which E_0 turns out to be smaller than the Laughlin energy. It is therefore reasonable to believe that for v almost equal to 1/9 a phase transition occurs and the 2DEG passes from a liquid to a crystalline phase. Moreover we notice that both the functions go to zero for $v \to 0$. This reflects the fact that the limit for small densities of both our and Laughlin models is a classical WC.

It is worthwhile to insist on the fact that the Wigner energy is a lower bound for a 2DEG system. This point has been discussed in [22] and in [13]. Here we only remind the same argument. Let Ψ_w be the N particle wave function corresponding to the Wigner crystal constructed with single particle δ-function orbitals centered in the triangular Wigner lattice and arranged in a single Slater determinant. Roughly speaking Ψ_w is an eigenstate of any local potential (Ψ_w does not belong to $\mathcal{L}^2(R^2 \otimes R^2 \otimes ....R^2)$). If V is our potential, $V = V_c + V_b$, that is the sum of the Coulomb electron interaction plus the background effect, then we have the following 'eigenvalue equation': $V \Psi_w = E_w \Psi_w$, E_w being the energy corresponding to the triangular Wigner lattice described by Ψ_w. Actually, Ψ_w is the ground state of V so that the inequality $<\Psi, V\Psi> \geq E_w$ holds for any normalized

function Ψ. So, if P is the operator that projects in the LLL, for any ϕ we can write

$$< \phi | \text{ PVP} | \phi > = < \text{P}\phi | \text{ V} | \text{P}\phi > \geq E_w$$

This implies that E_w is a lower bound for the ground state energy of PVP.

Going back to figure 3 we want to stress that the critical value we obtain essentially coincides with the one given by Levesque et al. in [21], that is with $V_0 = 1/9$. However there is still a certain difference with the experimental data reported in [9] where V_0 is obtained to be essentially 1/5. We will return on this point in Chapter 4, where some attempts will be made to approach this value.

We end this Chapter showing in figure 4 below the differences between $\Delta E_0(V)$ and $\Delta E^{CDW}(V)$ as obtained from (2.36) for the range of values of V for which both expansions make sense.
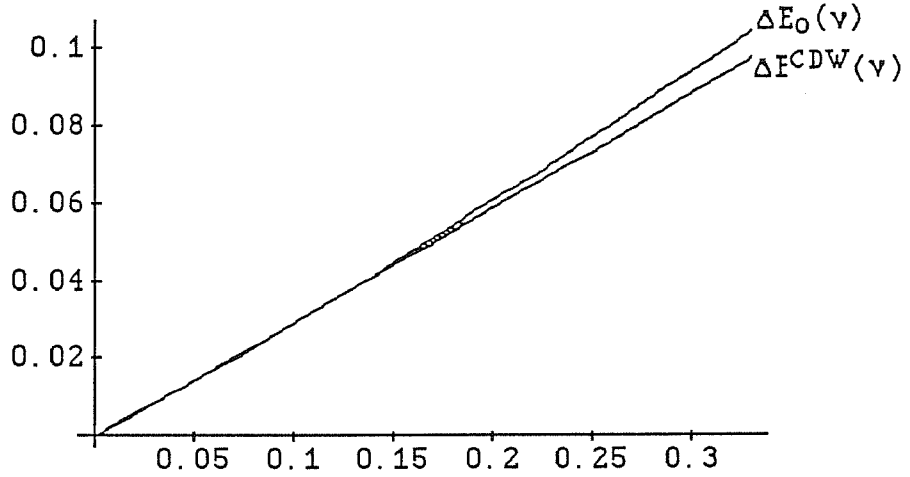

Fig.4

As we see the two functions look very much the same in this range of V. In particular they are almost identical for V less than 0.15, so that it is clear why our conclusions about the critical value of the filling coincide with the results discussed in [21] for a CDW state. The difference for $V >$ 0.15 are due to the fact that the function $E^{CDW}(V)$ gives only an approximation of the true value for $V = 1/3$ and $V = 1/5$ as we have already noticed. To be explicit, one can see that $E^{CDW}(V=1/3)$ is slightly minor than

the value explicitly computed. Moreover, at the same filling, our approximated energy $E_0(v)$ is slightly higher ($\sim$ 0.003 in our unities) than the true value given in (2.30), since we have obtained $E_0(v)$ neglecting the exchange term that for this value of v has a certain relevance being different from zero. However, in trying to obtain the same critical value of the filling given in [9], $v_0=1/5$, we do not need to add the exchange contribution in the expression of $E_0(v)$. In fact we have shown that it is of the order 10^{-4} or less for the relevant range of v. Therefore it does not modify much the form of $E_0(v)$ for $v<1/3$.

CHAPTER 3: LOCALIZATION AND ORTHOGONALITY

In this Chapter we will give some relevant results about the localizability of a wave function for a 2DEG starting from general considerations. The main tool we will use is the kq-representation, introduced first by Zak, see for instance reference [23], which is discussed in some details in Appendix 1. Using this quantum mechanical representation the orthogonality condition for functions of the first Landau level describing a $\nu = 1$ 2DEG is easily expressed and the general form of the solution is found. The related (x,y) wave function is obtained in [24] for a particular choice of the above solution, and an asymptotic decay of the $1/x$ kind is explicitly obtained. This behaviour is not due to the particular choice of the solution. We will show that it is a necessary consequence of the nature of the physical problem. Finally we extend some of the previous considerations to fillings different from one.

In the first part of this Chapter we restrict to a square two-dimensional lattice. In this way we maintain a simple notation that would be lost for different shapes of the crystal. However the triangular lattice will be briefly discussed at the end of the Chapter and we will show that no significant difference arises.

3.1: kq-Representation and Magnetic Translations

Here we want to diagonalize simultaneously the two operators $T(a_1)$ and $T(a_2)$ introduced in (1.5) in order to define a magnetic kq-representation. We will refer to Appendix 1 for notations and for the main ideas.

We recall that in Chapter 1 we have defined for our model two translation operators T_j commuting with the Hamiltonian $H_0 = \underline{\Pi}^2/2$ by the:

$$T(\underline{a}_j) = \exp\{ i \underline{\Pi}_c \cdot \underline{a}_j \} \qquad j=1,2 \tag{3.1}$$

where $\underline{\Pi}$ and $\underline{\Pi}_c$ in our unities are:

$$\Pi_x = p_x - y/2 \qquad \Pi_y = p_y + x/2 \tag{3.2}$$

$$\Pi_{cx} = p_x + y/2 \qquad\qquad \Pi_{cy} = p_y - x/2 \qquad\qquad (3.3)$$

The only non-zero commutation relations between the operators Π are:

$$[\,\Pi_y\,,\Pi_x\,] = [\,\Pi_{cx}\,,\Pi_{cy}\,] = i$$

from where it follows that

$$[\,H_0\,,\,T(\underline{a}_j)\,] = 0 \qquad\qquad j=1,2 \qquad\qquad (3.4)$$

Moreover we recall that the operators $T(\underline{a}_j)$ commute if the following condition is satisfied:

$$(\,\underline{a}_1 \wedge \underline{a}_2\,)_z = 2\pi \qquad\qquad (3.5)$$

In order to make explicit the characteristic of the operators Π to be conjugate operators we define two couples of such operators:

$$(Q,P) = (\Pi_{cx}\,,\Pi_{cy}) \qquad\qquad (3.6)$$

$$(Q^{\#},P^{\#}) = (\Pi_y\,,\Pi_x) \qquad\qquad (3.7)$$

They satisfy canonical commutation relations

$$[\,Q\,,P\,] = [\,Q^{\#}\,,P^{\#}\,] = i \qquad\qquad (3.8)$$

while all the other commutators are zero.
In these new variables we can rewrite

$$H_0 = \frac{1}{2}\,(P^{\#2} + Q^{\#2}) \qquad\qquad (3.9)$$

$$T_1 = \exp(iQa_1) \qquad\qquad T_2 = \exp(iPa_2) \qquad\qquad (3.10)$$

where the square nature of the lattice we are considering has been explicitated in the expressions defining the operators T_j.

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Being H_0 the Hamiltonian of a one-dimensional harmonic oscillator we know its ground state, which is the one describing the LLL. We choose to describe the complete wave function of the model in the P-$P^{\#}$ coordinate. Of course every other choice of variables, like, for instance, Q and $Q^{\#}$, would be equivalent to this one so that no particular physical and practical difference arises. Due to the independence of H_0 from the variables $Q^{\#}$ and $P^{\#}$ we can factor out the ground state in the form:

$$\Psi_0(P,P^{\#}) = <PP^{\#}| \Psi_0> = f_0(P^{\#})\, g(P) \qquad (3.11)$$

where $f_0(P^{\#})$ is the ground state of the Hamiltonian in (3.9)

$$f_0(P^{\#}) = \frac{1}{\pi^{1/4}}\, e^{-P^{\#2}/2}$$

and $g(P)$ can be any function of P, unless one introduces some extra constraints like, for instance, the orthogonality of the translated wave functions. This point will be widely discussed in Section 3.2, where we will show, following Zak, how the orthogonality request can almost fix the function $g(P)$.

Since we are interested in the asymptotic behaviour of Ψ_0 in the space of the coordinates we have to introduce the transformation rule between the P-$P^{\#}$-representation and the $\underline{r}$-representation. This formula has been discussed in references [24] and [27] and it has the following form

$$\Psi_0(x,y) = \frac{1}{2\pi} \int dP\, dP^{\#}\, e^{i(xy/2+xP^{\#}+yP+PP^{\#})}\, \Psi_0(P,P^{\#}) \qquad (3.12)$$

It is useful to stress that this explicit form strongly relies in the geometrical nature of the two-dimensional lattice. This point is reflected essentially in the definition of the canonical operators $Q,P,Q^{\#},P^{\#}$, see (3.6) and (3.7). In fact Q and P are, in general, defined by the scalar product $\underline{\Pi}_c \cdot \underline{a}_j$ and therefore their definition turns out to be very different for different shapes of the lattice, that is for different vectors of the basis $\underline{a}_j$. This implies that the relation between $\Psi_0(P,P^{\#})$ and $\Psi_0(x,y)$ is lattice-dependent. Such a dependence does not exist for the variables $Q^{\#}$ and $P^{\#}$ so that the form of H_0 is independent on the shape of the lattice. We will turn back on

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this point at the end of the Chapter where the definition of the conjugate operators Q and P for a triangular lattice is explicitly given and where it is shown that all the main statements below still hold for the triangular crystal.

Until now we have essentially made only a change of variables. Now we turn to kq-representation giving the form of the common set of eigenfunctions of the translation operators. We have, see Appendix 1,

$$f_{kq}(P) \equiv \, <P|\,kq> \, = \sqrt{\frac{a}{2\pi}} \sum_{n=-\infty}^{\infty} \delta(P-q-na) \, e^{-ikna} \qquad (3.13)$$

and its Fourier transform

$$f'_{kq}(Q) \equiv \, <Q|\,kq> \, = \sqrt{\frac{1}{a}} e^{ikq} \sum_{n=-\infty}^{\infty} \delta(k-Q+na) \, e^{iqna} \qquad (3.14)$$

It is useful to recall that for a square lattice the rationality condition (1.11) reads

$$a^2 = 2\pi \qquad (3.15)$$

(from where it follows that the over all constants in $f_{kq}(P)$ and $f'_{kq}(Q)$ coincide, since $a=2\pi/a$)

Let us now show the link between the PP# and the kq-representation. Using the completeness of the states $|kq>$, see [28], and equations (3.13) and (3.11) above we can write

$$g(P) = \int_{0}^{a} dk \int_{0}^{a} dq \, f_{kq}(P) \, C(k,q)$$

where we have defined $C(k,q) = \, <kq|\,\Psi_o>$. Expliciting the form of $f_{kq}(P)$ we finally deduce

$$g(P) = \sqrt{\frac{1}{a}} \int_0^a dk \ C(k,P-na) \ e^{-ikna}, \qquad P-na \in [0,a]$$

Following essentially the same steps but for the use of (3.14) instead of the (3.13) we obtain the Fourier transform of $g(P)$ as

$$g'(Q) = \sqrt{\frac{1}{a}} \int_0^a dq \ C(Q-na,q) \ e^{iqQ}, \qquad Q-na \in [0,a]$$

By changing variables in each of the two formulas above, $P \to P+na$ and $Q \to Q+na$, we obtain:

$$g(P+na) = \sqrt{\frac{1}{a}} \int_0^a dk \ C(k,P) \ e^{-ikna}, \qquad P \in [na,(n+1)a] \qquad (3.16)$$

$$g'(Q+na) = \sqrt{\frac{1}{a}} \int_0^a dq \ C(Q,q) \ e^{iqQ} \ e^{iqna}, \qquad Q \in [na,(n+1)a] \qquad (3.17)$$

We see that $g(P+na)$ can be interpreted as the n-th Fourier coefficient of the function of the k-variable $C(k,P)$ for any fixed P. Analogously $g'(Q+na)$ is the n-th Fourier coefficient of the function $C(Q,q)e^{iQq}$ interpreted as a function of the variable q, for any fixed Q.

We want to close this Section with a remark: in reference [23] Zak gives the following quasi-periodical boundary conditions for a generic function $C(k,q) = <kq|\Psi_o>$ in the kq-representation:

$$C(k+2\pi/a,q) = C(k,q)$$

$$C(k,q+a) = \exp(ika) \ C(k,q)$$

see also Appendix 1. In our opinion these do not hold true in general. The reason is that $g(P) = <P|\Psi_o>$ in (3.11) must be a function of $\mathcal{L}^2(R)$ and therefore it needs not to be in ℓ^1. This implies, see formula below and Appendix 1, that no change of index is allowed in the formula defining the kq-expression of the state Ψ_o starting from its r-representation:

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$$C(k,q) = \frac{1}{\sqrt{b}} \sum_{n=-\infty}^{\infty} \Psi_o(q-na) \, e^{ikna}$$

Therefore the second condition above is not valid in general and the boundary conditions assumed by Zak et al. only define a dense set in $L^2(R)$.

3.2: Orthogonalization

Let $C(k,q)$ be a generic function of the variables k and q. In reference [29] it has been shown that the operators T that define the representation become simple multiplication operators when applied to any function of k and q. Therefore the translated wave function is

$$C_{mn}(k,q) = \exp\{i(aqm + akn)\} \, C(k,q) \tag{3.18}$$

Orthogonality of the wave functions implies that two such functions at different sites have zero scalar product. Therefore for m and n not both equal to zero we require that:

$$\int dkdq \, C_{mn}(k,q)C^*(k,q) = \int dkdq \exp\{i(aqm+akn)\} \, |C(k,q)|^2 = 0 \tag{3.19}$$

where the integrations are extended from 0 to $2\pi/a=a$ in both variables. From (3.19) one deduces, through Fourier transform properties, that $|C(k,q)|^2$ must be a constant in k and q, so that the function $C(k,q)$ is a phase:

$$C(k,q) = A \, e^{i\tau(k,q)} \tag{3.20}$$

τ being a real function.

With the same Fourier-transform techniques it is easy to prove that the set $\mathcal{J} = \{C_{mn}(k,q), \forall \; m,n \text{ integers}\}$ is complete in $L^2([0,a]\otimes[0,a])$. This means that any function of this space orthogonal to all the C_{mn} is

necessarily equal to zero almost everywhere (a.e.). The proof is straightforward: if a function w(k,q) is orthogonal to all the $C_{mn}(k,q)$ for any n and m, then w*(k,q)C(k,q) must be zero a.e.. Moreover, being C(k,q) a phase, and therefore always different from zero, then w(k,q) = 0 a.e.. This proves the completeness of the set.

The orthogonality condition and the completeness of the set will be briefly analyzed in the case of filling different from 1 in Section 3.4, where the above results will be slightly modified.

3.3: Localization for $\nu = 1$

Here we collect all the informations obtained above and we prove a general theorem on the decay properties of the wave functions of the LLL of a 2DEG for filling equal to one.

First we compute the gaussian integration in $P^{\#}$ in (3.12) using the explicit form of $f_0(P^{\#})$. We get

$$\Psi_0(x,y) = \frac{e^{i(xy/2)}}{\sqrt{2}\pi^{3/4}} \int_{-\infty}^{\infty} dP \; e^{-(x+P)^2/2} \; g(P) \; e^{iyP} \tag{3.21}$$

Let us now fix the variable $y=y_0$. Forgetting about the inessential constants and neglecting the over all phases we find the following behaviour for the function $\Psi_0(x,y_0)$:

$$\Psi_0(x,y_0) \approx \int_{-\infty}^{\infty} dP \; e^{-P^2/2} \; g(P-x) \; e^{iy_0(P-x)}$$

and, if we fix $x=x_0$ and we use some easy properties of the convolutions we find

$$\Psi_0(x_0,y) \approx \int_{-\infty}^{\infty} dz \; e^{-z^2/2} \; g'(y-z) \; e^{ix_0(z-y)}$$

5 1

g' being the Fourier transform of the function g.

Since the convolution of a function F with a gaussian does not modifies the asymptotic behaviour of F we see from the above formulas that the x behaviour of Ψ_o is dictated by g while the y behaviour of Ψ_o is governed by g'. Explicitly we have:

$$\Psi_o(x,y_o) \approx g(-x) \qquad \Psi_o(x_o,y) \approx g'(y) \qquad (3.22)$$

These relations, together with formulas (3.16) and (3.17), show the connection between C(k,q) and Ψ_o for large values of x and y.

In order to study the decay of Ψ_o we will use some properties of the Fourier transforms. In reference [25] it is proven the following theorem:

- if a function f(x), together with its first n-1 derivatives is continuous and differentiable between 0 and $2\pi/a$ inclusive, and the n-th derivative is differentiable over the same interval except possibly a finite number of points $x=x_n$ where it may have bounded discontinuities, then the coefficients of its Fourier expansion approach zero at least as fast as k^{-n-1} as $k\to\infty$.

From this theorem and from the study of the Fourier coefficients of a discontinuous step, see again reference [25], it is straightforward to prove the following

Theorem
- If f(x) is a function defined in the interval $(0,2\pi/a)$ where it has at least one discontinuity, then the coefficients of its Fourier expansion approach zero as fast as k^{-1} as $k\to\infty$.

proof
The proof is based on the possibility of writing any function with a single discontinuity as the sum of a number of functions with a certain regularity plus a step function. In figure 5 we see this feature explicitly in an easy example where we show that $\forall\ x \in [a,b]$ it is possible to write

$$f(x) = f_1(x) + f_2(x) + s(x)$$

Here $f_1(x)$ and $f_2(x)$ have a discontinuity in $x=x_0$, and $s(x)$ is a step function with $\Delta = y_3-y_0$. Finally we have defined $\delta= -(y_3-y_2)$.
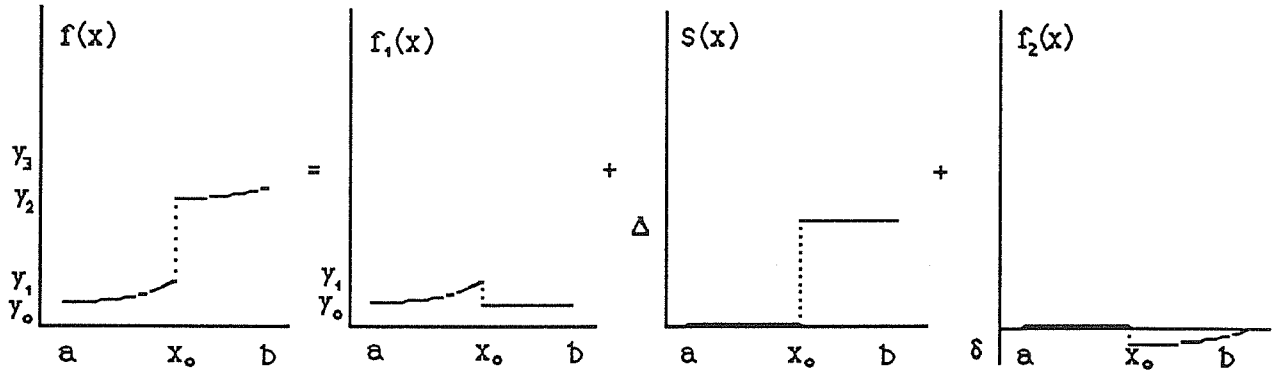

Fig.5

The asymptotic behaviour of the Fourier coefficients of $f_1(x)$ and $f_2(x)$ is governed from the previous theorem, so that they go both at least as k^{-1}. For what concerns the behaviour of the coefficients of the step function $s(x)$ this can be shown to be exactly of the k^{-1} form, so that the theorem is proven.

The next step consists in proving that or $C(k,q)$ or $\chi(k,q) =C(k,q)\ e^{ikq}$ must have at least one discontinuity respectively in k and in q in their respective domains. If this is true then, being $g(P+na)$ and $g'(Q+na)$ the Fourier coefficients of these functions, see (3.16) and (3.17), then g or g', or both, must decrease as n^{-1} due to the above theorem. Therefore, from (3.22) above, we derive that $\Psi_0(x,y_0)$ or $\Psi_0(x_0,y)$ have the predicted asymptotic behaviour. The theorem can be enunciated as follows:

Theorem
- It is impossible to have simultaneously $C(k,q)$ continuous in $k\in [0,2\pi/a]$ for any q fixed in $(0,2\pi/a)$ and $\chi(k,q)$ continuous in $q\in [0,2\pi/a]$ for any k fixed in $(0,2\pi/a)$.

proof:
Let us suppose, ab absurdo, that both continuities above are allowed. Then, since e^{ikq} is continuous in $(0,2\pi/a)\times(0,2\pi/a)$ and $\chi(k,q)$ is q-continuous by hypothesis, it follows that $C(k,q) = e^{-ikq}\ \chi(k,q)$ is also

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continuous for any $q \in (0, 2\pi/a)$ (beside being continuous for any $k \in [0, 2\pi/a]$). The values of $C(k,q)$ in $q=0$ and $q=a$ are naturally defined using the usual limiting procedure

$$C(k,0) = \lim_{q,0+} C(k,q)$$

$$C(k,a) = \lim_{q,a-} C(k,q)$$

which preserves the continuity in q of the function also on the boundary.

We conclude that the function $C(k,a)$ is obtained from $C(k,0)$ via a continuous deformation of it and therefore both functions belong to the same homotopy class.

On the other hand, continuity in q of the function $\chi(k,q)$ implies that

$$\lim_{q,a-} \chi(k,q) = \lim_{q,0+} \chi(k,q)$$

or, expliciting the form of χ,

$$C(k,a)\, e^{ika} = C(k,0)$$

Due to the fact that $|C(k,q)| = 1$ for any k and q inside the interval $[0,2\pi/a] \times [0,2\pi/a]$ (orthogonality condition), the above equality proves that $C(k,0)$ and $C(k,a)$ have different winding numbers. Therefore they cannot belong to the same homotopy class.

This ends the proof.

Let us now choose $C(k,q)$ to be discontinuous in k. From the first theorem we conclude that $\forall$ P fixed the function $g(P+na)$ is not in l^1 since it goes like $1/n$.

The same conclusion can be obtained using some easy considerations on the inverse Fourier transform of formula (3.16):

$$C(k,P) \approx \sum_n g(P+na)\, e^{ikna}$$

where an irrelevant constant has been neglected. If $g(P+na) \in l^1$ then the above series is uniformly convergent so that, $\forall$ P fixed, $C(k,P)$ is continuous

in k, which is in contrast with the hypothesis. Therefore the function g cannot be in ℓ^1.

The proof given here is different from the one proposed in [28] where, making use of the quasi-periodic boundary conditions, it is proven that any continuous function C(k,q) must have a zero in the kq-cell. Since orthogonality for filling one forces C(k,q) to be a phase, so that it is always non zero, they deduce that it must be necessarely discontinuous. No rigorous result concerning the asymptotic behaviour of the wave functions is given in [28].

3.4: Filling different from 1

The content of this section is essentially in the expression of the orthogonality condition (3.20) for a filling different from 1. We will discuss first the case of $v=1/2$ and then we state the condition for the more relevant filling $v=1/3$.

In order to discuss a square 2DEG with filling one half we can imagine to built up a lattice with a free lattice site between any two electrons. In this way the relevant set of functions, in the kq-representation, it is no longer the set $\mathcal{J}$ introduced before but it is only a subset of this, $\mathcal{J}'=\{\exp\{i(2inka+imqa)\}\ C(k,q),\ \forall\ m,n\ \text{integers}\}$. Let us now define two regions in the kq-unit cell D: $D_1=\{k\in[0,a/2],\ q\in[0,a]\}$, $D_2=\{k\in[a/2,a],\ q\in[0,a]\}$, so that $D = D_1 + D_2$. For any C(k,q) it is always possible to put

$$C(k,q) = C^{(1)}(k,q) + C^{(2)}(k,q)$$

with $C^{(i)}(k,q)$ such that $\text{supp}\{C^{(i)}(k,q)\} = D_i$, i=1,2.

We require that the functions of $\mathcal{J}'$ are still mutually orthogonal in the unit cell, D. We therefore require that

$$I = \int_D dkdq\ e^{2inka+imqa}\ |C(k,q)|^2 = 0 \qquad \forall\ m,n$$

This equation does not allow us to deduce that $C(k,q)$ is a phase since $e^{2inka+imqa}$ is not a Fourier basis of the unit cell, condition that is satisfied by the set $\{e^{inka+imqa}\}$. It is convenient to divide the above integral I into two pieces:

$$I= \int_{D_1} dkdq \ e^{2inka+imqa} |C(k,q)|^2 + \int_{D_2} dkdq \ e^{2inka+imqa} |C(k,q)|^2$$

In the second term above we change integration variable: $k \rightarrow k'= k - a/2$ so that the integration in k' is extended from 0 to $a/2$. Therefore we can rewrite I in the form

$$I= \int_{D_1} dkdq e^{2inka+imqa}|C(k,q)|^2 + \int_{D_1} dk'dq e^{2ink'a+imqa}e^{2in\pi}|C(k'+a/2,q)|^2$$

(we remind that $a/2 = \pi/a$) or

$$\int_{D_1} dkdq \ e^{2inka+imqa} \left\{ |C(k,q)|^2 + |C(k+a/2,q)|^2 \right\} = 0$$

Since $e^{2inka+imqa}$ is a Fourier basis in D_1, we can conclude that $C(k,q)$ must satisfy the following orthogonality condition:

$$|C(k,q)|^2 + |C(k+a/2,q)|^2 = 1 \qquad (3.23)$$

(1 has been chosen for simplicity. Actually every constant in k and q can be used instead of the unity) which, of course, admits also solutions that are not simple phases.

For what concerns the completeness of the set $\mathcal{J}'$ in $\mathcal{H}_{\nu=1}$ it is immediate to understand that this fails. In fact it is very easy to built up non zero functions that are orthogonal to all the functions of $\mathcal{J}'$.

Analogously to (3.23) for $\nu=1/2$ and to (3.20) for $\nu=1$ we get the following orthogonality condition for $\nu=1/3$ using the same techniques as before:

$$|C(k,q)|^2 + |C(k+\pi/3a,q)|^2 + |C(k+2\pi/3a,q)|^2 = 1$$

which shows again that solutions different from a simple phase are allowed, even for such a filling.

We conclude that the orthogonality condition for the kq-wave functions is filling dependent. Of course different solutions, which are no longer a phase, can give different localizations than the one obtained in the previous Section for a filling one 2DEG. This follows from the fact that the main theorem of the previous Section in general does not hold anymore.

3.5: Triangular lattice

As already anticipated the main difference among lattices with different shapes consists in the different definitions of the variables $Q, P, Q^{\#}$ and $P^{\#}$. In Section 3.1 we have defined, for a square lattice

$$(Q,P) = (p_x + y/2, \ p_y - x/2) \qquad (Q^{\#}, P^{\#}) = (p_y + x/2, \ p_x - y/2)$$

Now we use the definitions of Section 1.3:

$$(Q^{\#}, P^{\#}) = (p_y + x/2, \ p_x - y/2) \tag{3.24}$$

$$(Q,P) = (p_x + y/2, \ p_x/\sqrt{3} + y/2\sqrt{3} + p_y - x/2) \tag{3.25}$$

In [27] it is discussed in which way to construct the analogous of formula (3.12) for any linear canonical transformation. For such a change of variables we can write the following transformation rule:

$$\Psi_o(x,y) = \frac{e^{i/2[xy - y^2/\sqrt{3}]}}{2\pi} \int_{-\infty}^{\infty} dP^{\#} \ e^{ixP^{\#} - iP^{\#}y/\sqrt{3} - iP^{\#2}/2\sqrt{3}} \ .$$

$$\cdot \int_{-\infty}^{\infty} dP \ e^{iyP + iPP^{\#}} \ \Psi_o(P, P^{\#}) \tag{3.26}$$

Using the explicit form (3.11) of $\Psi_o(P,P^\#)$ we can perform the $P^\#$ gaussian integration. As it happens for the square crystal, to obtain the asymptotic behaviour of $\Psi_o(x,y)$ we get integrals that are essentially convolutions of $g(P)$ or of its Fourier transform with gaussian functions. Therefore the conclusions are totally identical to the ones that led to formula (3.22), namely, we still have:

$$\Psi_o(x,y_o) \approx g(-x) \qquad \Psi_o(x_o,y) \approx g'(y)$$

even for this lattice shape.

Of course, being all the other results of Section 3.3 lattice independent, no difference arises in the final conclusions and therefore, for equal values of the filling, the asymptotic behaviour of the electron wave function is the same of the one obtained for the square lattice.

CHAPTER 4: IMPROVED HARTEE-FOCK

In Chapter 2 a complete, rigorous, treatment of the WC through a perturbative Hartee-Fock procedure has been carried out. The results however cannot explain fully all the experimental data in [9] where a critical value of the filling, $v_0=1/5$, has been obtained. To get this value from a theoretical point of view it is natural to introduce some modifications on the trial ground state wave function since this is the main ingredient to build up the crystal phase of the 2DEG. A first indication of a critical filling near to 1/5 was already obtained in [30] where the absence of FQHE in high-mobility GaAs samples was interpreted as a Wigner crystallization. In [31] a modification of the wave function originally proposed in [7] was introduced through correlations between the electrons. This modified wave function allowed the authors to find a $v_0 \approx 1/7$. Here we want to use another approach. We still use a single Slater determinant but we change the single electron wave function. No complete energetic computation is performed but many ideas are discussed together with some numerical results that, in our opinion, give an exact idea of the effective modification in the ground state energy. In a second Section we will introduce another trial function looking promising for giving a real improvement of the energy E_0, on which some considerations will be discussed. Both these proposals are essentially dictated by physical arguments more than from mathematical reasons.

4.1: Polarization of the wave functions

The wave function $\Psi_{0,0}(x,y)$ which has been used in Chapters 1 and 2 to build up the Slater determinant has a spherical symmetry: it is invariant under any spatial rotations. When the electrons are considered in a triangular lattice it is, however, too optimistic to think that no modification is induced in the form of a single wave function as a consequence of the presence of the other electrons. On the contrary it is natural to expect that any electron slightly modifies the wave function of any other particle breaking in this way the original invariance for generic rotations of $\Psi_{0,0}$. What one could expect is that the true single-particle wave function still

maintains a certain invariance but only for rotations of multiples of 60°. In figure 6 below we show, not in the true proportions, how we expect that the original spherical symmetry can be modified by the mutual electron interaction.
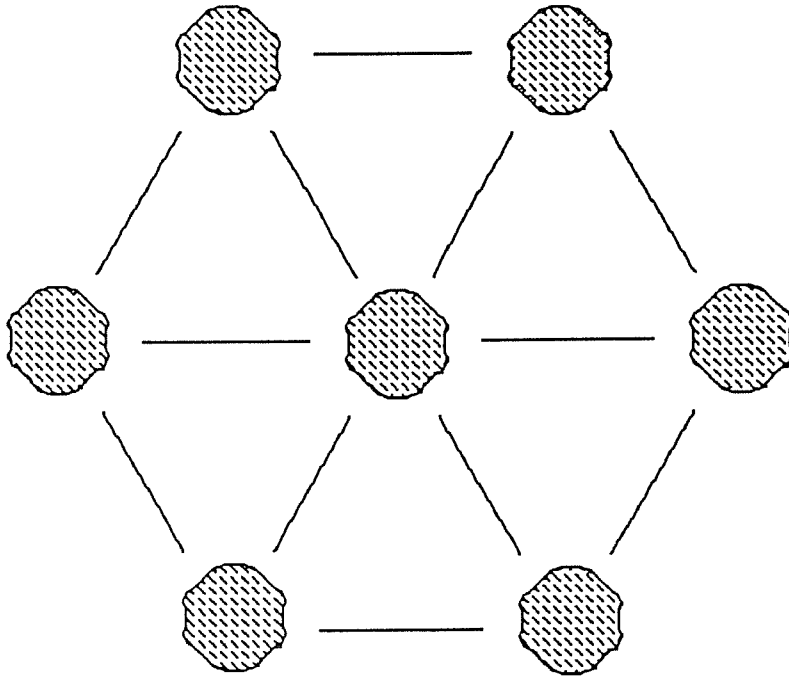

Fig.6

Of course, in order to describe such wave functions, we need to modify $\Psi_{0,0}$, keeping in mind that we do not want to go out of the LLL. In Chapter 1, formula (1.4), we have introduced a basis of such a Landau level, which we rewrite in the more convenient form

$$\Phi_m(z) = (2^{m+1}\pi \; m!)^{-1/2} \; z^m \exp[-|z|^2/4] \qquad (4.1)$$

with $z = x + iy$, [22].

We define a new wave function $\xi_0(z)$ as a linear combination of all the functions Φ_m. Then we impose to $\xi_0(z)$ to be invariant for rotations of 60°. In this way we will find some conditions on the coefficients defining ξ_0. We define:

$$\xi_0(z) = \sum_{n=0}^{\infty} d_n \Phi_n(z) \tag{4.2}$$

that is normalized if we assume that

$$\sum_{n=0}^{\infty} |d_n|^2 = 1 \tag{4.3}$$

Rotations of 60° imply that

$$z \rightarrow z' = \frac{1}{2}(1 - i\sqrt{3})\, z$$

so that the difference between the functions $\Phi_m(z')$ in the rotated variable and $\Phi_m(z)$ follows only from the presence of the z^m factor. We have

$$\Phi_m(z') = \left[\frac{1}{2}(1 - i\sqrt{3}) \right]^m \Phi_m(z)$$

Using this relation the invariance condition of the function $\xi_0(z)$, $\xi_0(z') = \xi_0(z)$, is expressed in a very simple way:

$$\sum_{m=0}^{\infty} d_m \Phi_m(z) \left\{ 1 - \left[\frac{1}{2}(1 - i\sqrt{3}) \right]^m \right\} = 0$$

Being the $\Phi_m(z)$ linearly independent functions we deduce that all the coefficients must be equal to zero. Since $[(1-i\sqrt{3})/2]^m = 1$ for $m = 0,6,12,..$, while it is different from 1 for any other m, we conclude that only the coefficients d_{6n}, n integer, can be different from zero. The generic wave function $\xi_0(z)$ belonging to the LLL and invariant for rotations of 60° has, therefore, the following expression:

$$\xi_0(z) = \sum_{n=0}^{\infty} d_{6n} \Phi_{6n}(z) \tag{4.4}$$

where the coefficients d_{6n} satisfy the normality condition deduced from (4.3).

All throughout this Section we will restrict the above summation only to the first two contributions:

$$\xi_0(z) = d_0 \, \Phi_0(z) + d_6 \, \Phi_6(z) \qquad (4.5)$$

$$|d_0|^2 + |d_6|^2 = 1 \qquad (4.6)$$

As for the standard procedure, we use the translation operators T_j to built up the various wave functions localized in the different lattice points. We define

$$\xi_{n,m}(z) = T_1^n \, T_2^m \, \xi_0(z) \qquad (4.7)$$

which can be written, using the $\underline{r}$-coordinate, as

$$\xi_{n,m}(\underline{r}) = (-1)^{nm} \, e^{i/2(Y_{n,m}x \, - \, X_{n,m}y)} \, \xi_0(\underline{r}- \underline{R}_{n,m}) \qquad (4.8)$$

where $\underline{R}_{n,m}$ has been defined in (1.15).

An interesting feature of these wave functions is that their overlap is absolutely equal to the one of the $\Psi_{n,m}$ functions. Explicitly, we have:

$$c'_{nm} = (\, \xi_{00}, \xi_{n,m}) = (-1)^{n_1 n_2} \, e^{-\underline{R}_n^2/4} = c_{nm} \qquad (4.9)$$

In finding this formula a series of gaussian integrations have been performed. We have also used condition (4.6) and the following integral given in [26]

$$\int_0^\infty e^{-\lambda x^m} \, x^k \, dx \; = \; \frac{1}{m} \, \lambda^{-\frac{k+1}{m}} \, \Gamma(\frac{k+1}{m})$$

where Γ is the Gamma function.

A set of orthonormal states of the LLL can be constructed in exactly the same way as in Chapter 2. Due to equation (4.9) we can write

$$\Omega_i \approx \xi_i - \frac{1}{2} \sum_{n \neq 0} c_n \, \xi_{i+n} + \frac{3}{8} \sum_n \overset{(s \neq n)}{\underset{s \neq 0}{\sum}} c_{n-s} \, c_s \, \xi_{i+n} \qquad (4.10)$$

We now observe the following points:

- $\Phi_m(z)$ describes a function that has a mean value of $\underline{r}$ larger for larger m, see [22]. This suggests that, if we choose as a trial ground state the function $\Phi_6(z)$ (or a small perturbation of this), and we perform an energy computation, the result we get would be, in principle, much bigger than the one found in Chapter 2, due to a minor distance among the electrons in the sample. As a matter of fact this computation can be done since it fits in our general approach. We have done it and we have found a result that confirms the above guess;

- the previous point suggests therefore that d_6 must be small compared to d_0. Therefore the passage from the function $\Phi_0(z)$ to the combination $\xi_0(z)$ would give a perturbation of the original result. We will estimate that this change in energy is of the same order of the non-orthogonality contributions $\delta E_d + \delta E_s$ introduced in Chapter 2. Moreover, since the changes in $\delta E_d + \delta E_s$ due to the polarization effects are essentially perturbations of the second order, we neglect such contributions in the computation of E_0.

In order to analyze the energetic behaviour of $\xi_0(z)$ and of the related Slater determinant, we have compared $\sum E_d(i,0)$ with the analogous contribution $\sum E'_d(i,0)$ obtained by substituting $\xi_0(z)$ to $\Psi_0(z)$ in formula (2.17). We define:

$$E'_d(i,j) = \left(\int d^2\underline{r_1} \; d^2\underline{r_2} \; \frac{|\Omega_i(\underline{r_1})|^2 \, |\Omega_j(\underline{r_2})|^2}{|\underline{r_1} - \underline{r_2}|} \right)_{c_n = 0} \qquad (4.11)$$

so that we have

$$E'_d(i,0) = \int d^2\underline{r}_1 \, d^2\underline{r}_2 \, \frac{|\xi_i(\underline{r}_1)|^2 \, |\xi_0(\underline{r}_2)|^2}{|\underline{r}_1 - \underline{r}_2|} \tag{4.12}$$

The change in energy due to the exchange contribution is some order of magnitude less that the one given by the direct term. Therefore it will be neglected in our estimate.

The explicit computation is sketched in Appendix 4. Of course we must use expressions (4.5) and (4.8) in formula (4.12). In this way we get nine contributions that can all be conducted to a single integral:

$$I = \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, e^{-\alpha(\underline{r}_2 - \underline{R}_2)^2/2} \, e^{-\beta(\underline{r}_1 - \underline{R}_i)^2/2}$$

which has been exactly computed with analogous techniques as the ones used in Appendix 2.

However in Appendix 4 a further difficulty of this computation will be explicitated, namely the need of computing high derivatives of the modified Bessel function I_0. This will force us to use an asymptotic expression for the integral I, analogous to the one obtained for the matrix element V_{ijkl}. Of course in order to have meaningful informations about the energetic improvement we must compare the result we get with the one obtained in the "standard" approach in the same approximation, that is using the same expansion for I_0. We believe that, in spite of all the approximations we are forced to introduce, the conclusions we get have a real interest since they allow to obtain conclusive informations about the effective improvement given by the approach here proposed.

We compare the following quantities for a $v=1/3$ lattice:

$$E_p = \frac{1}{2} \sum_{i \neq 0} \left[E_d(i,0) - \frac{1}{|R_i|} \right] \tag{4.13}$$

with the modified one

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$$E'_p = \frac{1}{2} \sum_{i \neq 0} \left[E'_d(i,0) - \frac{1}{|R_i|} \right] \qquad (4.14)$$

which in Appendix 4 is proven to be of the form

$$E'_p = \frac{1}{2} \sum_{i \neq 0} \left\{ (1+6|d_6|^2) \frac{1}{|R_i|^3} + \frac{1}{2\sqrt{6!}} Re \left[d_0 * d_6 \frac{1}{\eta_1 *^6} \right] * \right.$$

$$* \left(\frac{11!!}{|R_i|} + (1+3|d_6|^2) \frac{13!!}{|R_i|^3} \right) + \frac{1}{2^5 6!} Re \left[d_0 *^2 d_6^2 \frac{1}{\eta_1 *^{12}} \right] \left(\frac{23!!}{|R_i|} + \frac{25!!}{|R_i|^3} \right) +$$

$$\left. + \frac{1}{2^5 6!} |d_0|^2 |d_6|^2 \left(\frac{(11!!)^2}{|R_i|^{13}} + \frac{(13!!)^2}{|R_i|^{15}} \right) \right\} \qquad (4.15)$$

Here we have defined $(2n+1)!! = 1 \cdot 3 \cdot 5 \cdots (2n-1) \cdot (2n+1)$ and $\eta_1 = X_i + i Y_i$ is the complex form of the lattice vector $\underline{R_i}$.

From the above formula we see that if d_6 is zero then E'_p reduces to E_p when expressed in the same approximation, that is

$$E'_p(d_6=0) = \frac{1}{2} \sum_{i \neq 0} \frac{1}{|R_i|^3}$$

while if d_0 is zero (and therefore, due to condition (4.6), $|d_6|=1$) then

$$E'_p(d_0=0) = \frac{7}{2} \sum_{i \neq 0} \frac{1}{|R_i|^3}$$

which is 7 times the standard result. This first observation proves our original claim about the perturbative rôle of $\Phi_6(z)$ in the definition of the new function $\xi_0(z)$.

The main point consists now in trying to find the absolute minimum of E'_p as a function of the complex quantities d_0 and d_6. We have assumed for simplicity real values for d_6 since it is sufficient, see (4.15), to have a

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single complex coefficient. We have found the, hopefully, absolute minimum of E'_p for:

$$d_0 = 0.9998 \exp(i\pi) \qquad\qquad d_6 = |d_6| = 1 - |d_0|^2 \qquad (4.16)$$

in correspondence of which we found the following value of E'_p

$$E'_p = 0.0541 \qquad\qquad\qquad (4.17)$$

which must be compared with the corresponding value of E_p, that is $E_p = 0.0542$.

We see that the difference between the two is exactly of the same order as the non-orthogonality contribution δE_d, that is very small and not so significant to make one believes that $\xi_0(z)$ is the correct wave function for the FQHE. Moreover from (4.15) it is easy to verify that the dependence on v is still analytical: no cusp in the energy appears.

Therefore we conclude this Section observing that a polarization mechanism, although being natural and physically unavoidable, is too weak to significantly lower the energy of the 2DEG.

4.2: Better localization of the wave function

We consider in this Section a filling one third 2DEG. The main idea for constructing a new trial function is essentially to go out from the relevant Hilbert space $\mathcal{H}_{v=1/3}$ (but not from the LLL). The reason is the following: in a system with N electrons and N vectors basis only one antisymmetric wave function can be constructed; this implies that we do not really change the complete wave function if we build up Λ_0 with the functions Ψ_n or with any linear combinations of them. This explains why our results are not significantly different from the ones given by Maki & Zotos, [7]. Any numerical difference between our approaches is due not to real inequivalence between the two methods but only to the different approximations considered. We therefore need to go out from the Hilbert space $\mathcal{H}_{v=1/3}$ generated by the functions Ψ_n (or Ω_n) localized around the various lattice sites, for trying to improve significantly the Hartee-Fock approximation.

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It is at this level that the sublattice approach introduced in Section 2.1 assumes a certain relevance: in figure 7 the lattice sites occupied for a $v = 1/3$ 2DEG minimal lattice are marked.
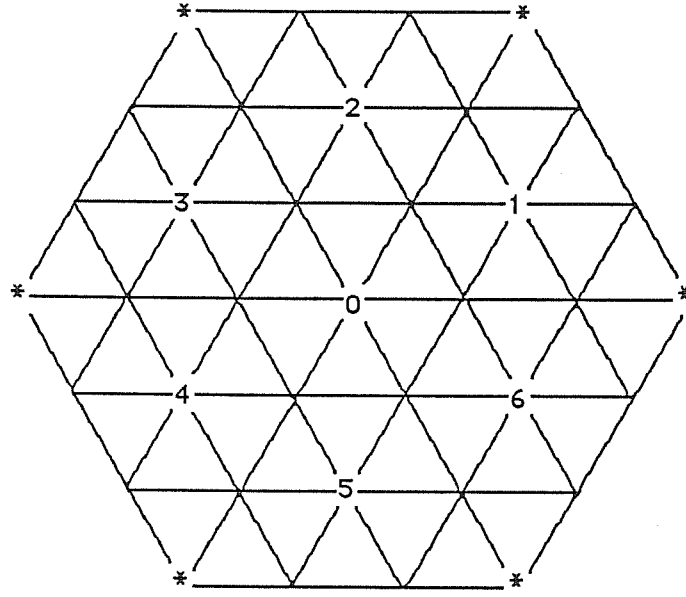

Fig. 7

We see that each occupied site is encircled by 6 free sites. We can think to paste to each of these sites an electron wave function, even if such function does not belong to $\mathcal{H}_{v=1/3}$. The physical idea is that a new wave function can be constructed using these extra-functions as a sort of screen for the electron placed in the centre of the circle:

$$\xi_0(\underline{r}) = N \left[\Psi_0(\underline{r}) + \sum_{n}^{f.s.} \alpha_n \Psi_n(\underline{r}) \right] \qquad (4.18)$$

where f.s. stands for 'first shell'. We mean that the summation must be extended only to the first shell of the minimal lattice encircling the site $(0,0)$. N is the normalization constant that is, obviously, a function of the complex coefficients α_n.

An easy symmetry consideration shows that $|\alpha_n|$ must be independent of the related site of the first shell. An estimate of the arguments of α_n can be found requiring that the function $\xi_0(\underline{r})$ satisfies the following "screening condition": we require that in all the sites of the first shell around the origin the value of $\xi_0(\underline{r})$ is almost zero. This suggests that the overlap

between two "screened" functions of $\mathcal{H}_{v=1/3}$ would be minor than the standard c_n due to a better localization of the electron wave functions.

In order to study the possible values of the coefficients α_n we put

$$\alpha_n = \alpha\ e^{i\varphi_n} \qquad\qquad (4.19)$$

α being equal to $|\alpha_n|$.

From the condition

$$\xi_0(\underline{r}) \approx 0 \quad \forall\ \underline{r} \text{ of the first shell} \qquad\qquad (4.20)$$

we obtain a system of six equations, which gives an approximate value of the coefficients α_n. Solving the system we get

$$\alpha_n \approx -0.2418 \qquad \forall\ n \qquad\qquad (4.21)$$

This result is, of course, only orientative; however it gives a feeling that not only the modulus but also the phases are independent of the lattice index n.

Actually, it is easy to prove that the natural guess of a better localization of the function $\xi_0(\underline{r})$ in (4.18) with respect to the one of $\Psi_0(\underline{r})$ is essentially wrong. This is due to a general property of the gaussian functions that is easily proved ucing the magnetic variables defined in (3.6) and (3.7). It is easier to use the square lattice to simplify the computation. If we write $\underline{r}^2$ in terms of Q, P, $Q^\#$, $P^\#$ and we compute its mean value in a generic state $\eta(\underline{r})$ of the LLL it is easy to prove that the minimum of $< \underline{r}^2 >$ is obtained if $\eta(\underline{r}) = \Psi_0(\underline{r})$. Since, moreover, the mean value of $\underline{r}$ is zero for any function $\eta(\underline{r})$ with the same simmetry of the lattice we conclude that $\Psi_0(\underline{r})$ has a better localization than any of the $\xi_0(\underline{r})$.

The above result does not imply that the ground state energy cannot be lowered; it only says that the quadrupole contribution in the expansion of the Coulomb potential cannot be improved using the linear combination in (4.8). A negative contribution to the ground state energy can follow however from the other multipoles in the expansion. This point must however still be checked.

From a practical point of view the computation of the ground state energy is, in principle, immediate. This follows from the fact that <u>all</u> the

integrals entering the expression of E_0 are of the well known form V_{ijkl} given in Appendix 2, so that their exact computations can be performed with no particular difficulty. Nevertheless the asymptotic behaviours need much cure since it is often not so easy to compute the signs of the various $Re[\underline{v}_c^2]$, already for a single matrix element. This is the reason why further studies are required in order to simplify as much as possible the energy computation. This is the scope of our further investigations.

CHAPTER 5: 2DEG AND SPIN MODELS

Here we analyze the link between the 2DEG in the LLL introduced in Chapter 2 and the Ising model with a long range interaction that has been discussed in reference [32]. We will first recall some of the results given in [32] and then we show how a Coulomb interaction Hamiltonian with no kinetic term can be written, in a first approximation, as the Hamiltonian of this Ising model.

Before starting with this analysis we want to recall that spin systems have played a very crucial rôle in recent years for obtaining many physical results since they often give a simplified form of a much more complex system. The first model that comes in mind is, obviously, the BCS model of superconductivity in the Anderson's language, see, for instance, reference [33]. More, even High Tc-Superconductivity is believed to be described by spin models like the Hubbard one. This, in the limit of large U and for half-filling, turns out to be approximated by an Heisemberg anti-ferromagnetic model with interaction restricted only to the nearest sites.

For what concerns the FQHE some spin models have been proposed, for instance, by Kivelson et al. in [17], even if no definitive sentence has been made up to now in our knowledge.

5.1: Long Range Interaction Ising Model

In [32] we have discussed in which sense the infinite volume limit of an Ising model described by the following finite volume Hamiltonian

$$H_V = - \sum_{ij \in V} J_{ij} (\sigma_3^i - \sigma')(\sigma_3^j - \sigma') \qquad (5.1)$$

can be defined. Here σ' has the physical meaning of an uniform background and it is assumed to be $|\sigma'| \leq 1$. We stress that σ' must not be confused with the positive background we added to the electron system for obtaining a finite energy. In (5.1) we have assumed that the potential is symmetric, $J_{ij} = J_{ji}$, and off diagonal, $J_{ii} = 0$.

As long as V is keepen finite, H_V belongs to the C*-algebra of the spin matrices $\mathcal{A}_V$ and therefore to the norm closure $\mathcal{A}$ of $U_V \mathcal{A}_V$. Since H_V is in $\mathcal{A}_V$,

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the Hamiltonian (5.1) defines a one parameter group of automorphisms of $\mathcal{A}_V$ by:

$$A \rightarrow \alpha_V{}^t(A) \equiv \exp(iH_V t) \, A \, \exp(-iH_V t) \qquad (5.2)$$

The automorphism $\alpha_V{}^t$ is called the algebraic dynamics of the model.

For lattice models with short range interactions the limit for $V \rightarrow \infty$ of $\alpha_V{}^t(A)$ exists in the norm topology of $\mathcal{A}$ and defines a group of automorphisms of $\mathcal{A}$ (see reference [34]). Norm convergence does not hold, however, for the dynamic defined by Hamiltonian (5.1), if the potential J_{ij} does not satisfy special regularity conditions. In particular in [35] the norm limit of $\alpha_V{}^t$ is shown to exist for summable J_{ij}. In [32] we have considered a potential that does not satisfy this condition so that the norm limit of $\alpha_V{}^t(A)$ does not exist in general.

The natural way for studying the thermodynamical limit consists in making reference to a family of 'relevant' states $\mathcal{F}$, [34] and [36], defining a strong topology in which the infinite volume limits exist. Of course the choice of the family of states is essentially dictated from the form of the potential: roughly speaking we can say that the more irregular the potential is the more regular need to be the states, or, better, that a slow decay of the potential at large distances must be balanced by a high regularity of the states in the same limit.

In particular if the family $\mathcal{F}$ we consider is made up only of product states that definitively point in the z-direction then strong convergence of the algebraic dynamics automatically follows. We only need to have the usual generic $|i-j|^{-m}$ behaviour, with $m>0$, of the potential J_{ij}. We have proven in [32] that σ' is actually a variable at infinity, that is, roughly speaking, the strong limit of the ergodic mean of the σ_3 spin operator, and that in the GNS-representations defined by the states in $\mathcal{F}$ it can assume only the values ± 1. In particular we have $\sigma' = +1$ if the product state definitively points in the up direction, while $\sigma' = -1$ if it points in the down direction.

The situation is under control even for $\underline{n}$-pointing product states. Let (n,θ,φ) be the spherical coordinates of the vector $\underline{n}$. We have proven that, if J_{ij} is such that

$$\sum_i J_{ij}{}^2 < \infty$$

then again the thermodynamical limit of the finite volume dynamics $\alpha_V{}^t$ exists in the ultrastrong topology defined by a family $\mathcal{F}$ of product states pointing in this generic direction $\underline{n}$. Again the values of σ' are fixed by the phase we are considering, that is, by the state used for the GNS-construction. In particular we have $\sigma' = \cos(\theta)$.

We can conclude that for any form of the potential it is possible to find a family of relevant states defining a topology in which we can define $\alpha^t \equiv \tau_{\mathcal{F}}\text{-}\lim_{V\to\infty} \alpha_V{}^t$. This turns out to be an automorphisms of the von Neumann algebra obtained by closing the C*-algebra $\mathcal{A}$ in the weak topology defined by $\mathcal{F}$.

5.2: Ising model and 2DEG

We will show here that the Ising model of the previous Section is a good candidate to describe, at a first order and for small fillings, a 2DEG in the LLL.

The starting point is the Coulomb interaction between the electrons in a strong magnetic field B. We assume B strong enough to force all the electrons in the LLL, so that the kinetic term, being a constant, can be neglected. We have, for an N-electrons system,

$$H_N = \frac{1}{2} \sum_{\substack{i \neq j}}^{N} \frac{1}{|\underline{r}_i - \underline{r}_j|}$$

that, in the second quantization language, becomes:

$$H_N = \frac{1}{2} \sum_{ijkl}^{N} W_{ijkl}\, a_i{}^* a_j{}^* a_l a_k \tag{5.3}$$

where we have defined the following matrix elements

$$W_{ijkl} = \int \frac{d^2\underline{x}\, d^2\underline{y}}{|\underline{x} - \underline{y}|} \Omega_i{}^*(\underline{x})\, \Omega_j{}^*(\underline{y})\, \Omega_k(\underline{x})\, \Omega_l(\underline{y}) \tag{5.4}$$

which satisfy the condition $W_{ijkl} = W_{jilk}$.

We stress that the functions Ω we are using are the orthonormalized ones, the ones we have introduced in Section 2.3, formula (2.13). They satisfy up to corrections of the 10^{-7} order to the orthogonality condition (2.14), which now we write simply

$$(\Omega_o, \Omega_n) = \delta_{n,o} \tag{5.5}$$

This condition implies that the a_i operators in (5.3) are canonical, so that they satisfy

$$\{ a_i, a_j{}^* \} = \delta_{ij} \tag{5.6}$$

and all the other anticommutators are zero.

This condition, again valid up to negligible corrections, would not be correct if we had used the not orthogonal functions Ψ in (1.14) since the corrections, that can be neglected here, would be of the 10^{-1} order.

To obtain the terms that give the biggest contributions to the approximate Hamiltonian H' we want to define, we write in an extended form the multiple summation in (5.3). Therefore we consider the contributions of the sum with all the four indexes equal, three equal and one different, two equal and two different and so on.

Using the nihilpotence of the fermion operators a_j and the symmetry of the W_{ijkl} matrix elements for exchange of indexes given above we can rewrite the Hamiltonian (5.3) in the form:

$$H_N = \frac{1}{2} \sum_{ij}^{N}{}'[W_{ijij}\, a_i{}^*a_j{}^*a_ja_i + W_{ijji}\, a_i{}^*a_j{}^*a_ia_j] + \sum_{ijk}^{N}{}'[W_{ijik}\, a_i{}^*a_j{}^*a_ka_i +$$

$$+ W_{ijki}\, a_i{}^*a_j{}^*a_ia_k] + \frac{1}{2} \sum_{ijkl}^{N}{}'W_{ijkl}\, a_i{}^*a_j{}^*a_la_k \tag{5.7}$$

where the primes in the summations indicate that all the indexes involved are different.

Let us now introduce the typical single mode number operator n_i:

$$n_i = a_i{}^*a_i \tag{5.8}$$

We can rewrite the above Hamiltonian as

$$H_N = \frac{1}{2} \sum_{ij}{}'[W_{ijij} - W_{ijji}]\, n_i\, n_j + \sum_{ijk}{}'[W_{ijik} - W_{ijki}]\, n_i\, a_j^*\, a_k +$$

$$+\frac{1}{2} \sum_{ijkl}{}'W_{ijkl}\, a_i^*a_j^*a_l a_k \qquad\qquad (5.9)$$

The hope is that we can split this Hamiltonian in a piece that would contain almost all the physics of the problem and in a small perturbation of it. We need, therefore, to estimate the matrix elements appearing in (5.9). We already know, from the estimates of Chapter 2, that the non orthogonality contributions are numerically meaningless. Therefore, to study the behaviour of the matrix elements in (5.9), we can use the approximation in which all the coefficients c_n are zero. This implies, due to definition (2.13), that $\Omega_i = \Psi_i$. In this approximation we have

$$W_{ijkl} = \int \frac{d^2x\, d^2y}{|\underline{x} - \underline{y}|}\, \Psi_i^*(\underline{x})\, \Psi_j^*(\underline{y})\, \Psi_k(\underline{x})\, \Psi_l(\underline{y})$$

which, together with (2.23), says that $W_{ijkl} = V_{ikjl}$.

We use the asymptotic behaviour obtained in Appendix 2 in order to study the relative weight of the various contributions of (5.9) and the estimate (A2.8) given in the same Appendix, which shows that, but for an inessential constant,

$$|V_{ijkl}| \le e^{-\frac{1}{4}(A_1 + A_2)}$$

where $A_1 = (\underline{R}_i - \underline{R}_j)^2/2$ and $A_2 = (\underline{R}_k - \underline{R}_l)^2/2$. We have:

i) $\qquad W_{ijij} = V_{iijj} \approx \dfrac{1}{|\underline{R}_i - \underline{R}_j|} \left\{ 1 + \dfrac{1}{|\underline{R}_i - \underline{R}_j|^2} \right\}$

ii) $\qquad |W_{ijji}| = |V_{ijij}| \le e^{-(\underline{R}_i - \underline{R}_j)^2/4}$

iii) $\qquad |W_{ijik}| = |V_{iijk}| \leq e^{-(\underline{R}_k-\underline{R}_j)^2/8}$

iv) $\qquad |W_{ijki}| = |V_{ikji}| \leq e^{-[(\underline{R}_i-\underline{R}_k)^2+(\underline{R}_i-\underline{R}_j)^2]/8}$

v) $\qquad |W_{ijkl}| = |V_{ikjl}| \leq e^{-[(\underline{R}_i-\underline{R}_k)^2+(\underline{R}_l-\underline{R}_j)^2]/8}$

From the above estimates it seems reasonable to define an unperturbed Hamiltonian H_0

$$H_0 = \frac{1}{2} \sum_{ij}{}' W_{ijij}\, n_i\, n_j \qquad\qquad (5.10)$$

and a perturbation δH

$$\delta H = -\frac{1}{2} \sum_{ij}{}' W_{ijji}\, n_i\, n_j + \sum_{ijk}{}'[W_{ijik} - W_{ijki}]\, n_i\, a_j{}^*\, a_k +$$

$$+ \frac{1}{2} \sum_{ijkl}{}' W_{ijkl}\, a_i{}^* a_j{}^* a_l a_k \qquad\qquad (5.11)$$

Of course this approximation is certainly wrong for filling near to 1 for the same reason for which it does not make sense to use the perturbative approach introduced in Chapter 2 for such a filling: the sum of the six terms coming from a single shell in δH can be of the same order of H_0. On the contrary, the smaller the filling is, the smaller are the coefficients appearing in δH, so that the separation of H into two terms seems to be meaningful. Of course we still don't know if H_0 contains the physics of the FQHE. This is absolutely a non trivial question that is still to be answered.

Let us now make a step forward, introducing spin variables in the game. Let $\Phi(n_1,......,n_N)$ be the eigenfunction of a 2DEG with N electrons satisfying the following equation:

$$n_i\, \Phi(n_1,..,n_i,...,n_N) = \Phi(n_1,......,n_N) \qquad \text{if } n_i = 1$$

$$ \qquad\qquad (5.12)$$

$$n_i\, \Phi(n_1,..,n_i,...,n_N) = 0 \qquad \text{if } n_i = 0$$

From the above equation it is immediate to verify that the operator defined as $-1+2n_i$ behaves like a σ_3^i operator when it acts on the Φ wave functions. In turns these can be interpreted as up or down spinors. We put:

$$\Phi(n_1,..,n_i=1,...,n_N) = \alpha_i$$

$$\Phi(n_1,..,n_i=0,...,n_N) = \beta_i \qquad (5.13)$$

$$-1+2n_i = \sigma_3^i$$

With the above position and with the definition

$$U_{ij} \equiv V_{ijij} = U_{ji} \qquad (5.14)$$

we can rewrite H_0 in the form

$$H_0 = \frac{1}{8} \sum_{ij}^{N}{}' U_{ij}\sigma_3^i\sigma_3^j + \frac{1}{4} \sum_{ij}^{N}{}' U_{ij}\sigma_3^i \qquad (5.15)$$

On the other hand the Ising Hamiltonian (5.1) can be rewritten, neglecting an irrelevant c-number, as:

$$H_v = - \sum_{ij \in V} J_{ij}\, \sigma_3^i\, \sigma_3^j + 2\sigma' \sum_{ij \in V} J_{ij}\, \sigma_3^i \qquad (5.16)$$

which has the same form of H_0 if

$$\sigma' = -1 \qquad \text{and} \qquad J_{ij} = - \frac{U_{ij}}{8} \qquad (5.17)$$

Since for such value of σ' no condition needs to be imposed on the potential to ensure the existence of the thermodynamical limit of the algebraic dynamics, see the previous Section and reference [32], we can conclude with the following claim:
-the Hamiltonian of a finite volume 2DEG with no kinetic term can be approximated, for small fillings, with an Ising Hamiltonian with a long range interaction. The algebraic dynamics given by this Hamiltonian exists

in any representation defined by product states that are local modification of a down state.

The next step would consist in trying to extract from this model some physical information to verify the real link between the Ising model and the FQHE or, at least, the 2DEG in the WC phase. We stress again that this is not a trivial step since it is by no means sure that all the relevant physics is contained in what we have called the "unperturbed Hamiltonian".

APPENDIX 1: kq-REPRESENTATION

In reference [23] J. Zak introduces two operators T(a) and T(b) that look very similar to the translations operators T_j we have defined in Chapter 2. They are

$$T(a) = \exp(ipa) \qquad T(b) = \exp(ixb) \qquad \text{(A1.1)}$$

satisfying the following condition:

$$ab = 2\pi \qquad \text{(A1.2)}$$

and where x and p are conjugate operators, $[x,p]=i$.

These are, due to condition (A1.2), two commuting operators. More, in reference [37] it is shown that they form a complete set of commuting operators. This means that any operator that commutes with both of them is necessarily a function of T(a) and T(b). Moreover for T(a) and T(b) we can find common eigenstates, Ψ_{kq}. They satisfy the following eigenvalue equations:

$$T(a)\Psi_{kq} = e^{ika} \Psi_{kq} \qquad T(b)\Psi_{kq} = e^{iqb} \Psi_{kq} \qquad \text{(A1.3)}$$

where k and q, called the quasimomentum and the quasicoordinate, vary respectively between 0 and $2\pi/a$ and 0 and $2\pi/b$. The explicit form of such eigenfunctions is given in the x-representation for instance in [37]:

$$\Psi_{kq}(x) \equiv < x \mid \Psi_{kq} > = \frac{1}{\sqrt{b}} \sum_{n=-\infty}^{\infty} \delta(x-q-na)\, e^{ikna} \qquad \text{(A1.4)}$$

while the p-representation of the same eigenfunction, that is the Fourier transform of (A1.4), $< p \mid \Psi_{kq} >$, is

$$\Psi_{kq}(p) \equiv \frac{e^{-ikq}}{\sqrt{a}} \sum_{n=-\infty}^{\infty} \delta(p-k-nb)\, e^{-iqnb} \qquad \text{(A1.5)}$$

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In finding this result it has been used an interesting property of the δ-function that is worthwhile to remember, that is:

$$\sum_{n=-\infty}^{\infty} \exp\left\{i \frac{2\pi}{c} n x\right\} = c \sum_{n=-\infty}^{\infty} \delta(x - nc)$$

Being eigenfunctions of a complete set of commuting operators, the functions Ψ_{kq} form a complete system of functions, satisfying the following orthogonality and closure relations, [28]:

$$\int \Psi_{kq}^{*}(x)\Psi_{k'q'}(x)\, dx = \sum_{m} \delta(k-k'-mb) \sum_{n} \delta(q-q'-na) \qquad \text{(A1.6)}$$

$$\int \Psi_{kq}^{*}(x)\Psi_{kq}(x')\, dkdq = \delta(x - x') \qquad \text{(A1.7)}$$

The labels k and q define the functions $\Psi_{kq}(x)$ completely (up to a phase factor), meaning that the coordinates k and q define a quantum-mechanical representation, called the kq-representation.

It is possible, but useless for our needs, to extend all the above formulas to more dimensions. Such a generalization can be found, for instance, in [23].

The main feature of the kq-representation is in the simultaneous use of partial information about both the coordinate and the momentum. By measuring k and q one can tell where in the unit cell of kq-space the values of the operators are but not in which of the cells they are. This is a consequence of the meaning of quasicoordinate and quasimomentum: k and k + 2π/a define the same eigenvalue of the operator T(a) and the same holds true for q and q + 2π/b for what concerns T(b). (In more dimensions we can add to the vectors k̲ and q̲ any vector of the reciprocal lattice). The knowledge of k and q leads only to partial information of the momentum and the coordinate and there is no violation of the uncertainty principle.

We give now the link between the r- and the kq- representations. Given a state ϕ of the Hilbert space this can be represented, for instance, as $\phi(x) = \, < x|\phi >$ or as $\phi(kq) = \, < kq|\phi >$. We have:

$$\phi(kq) = \int dx \; <kq|x><x|\phi> = \frac{1}{\sqrt{b}} \sum_{n=-\infty}^{\infty} \phi(q-na) \, e^{ikna} \qquad (A1.8)$$

while the inverse transform is

$$\phi(x) = \int dkdq \; <x|kq><kq|\phi> = \int dkdq \; \Psi_{kq}(x)\phi(kq) \qquad (A1.9)$$

The last point we want to mention here is the following: Boon and Zak in [28] give for $\phi(kq)$ the following boundary conditions:

$$\phi(k+2\pi/a,q) = \phi(kq) \qquad (A1.10)$$

$$\phi(k,q+a) = \exp(ika) \, \phi(kq) \qquad (A1.11)$$

which in our opinion are not totally correct. In fact condition (A1.11) is derived from (A1.8) by a change of index in the summation, change which is allowed only for ϕ in l^1. Since our Hilbert space is of course an $L^2(R)$ space that is not contained in l^1, then not all the relevant wave functions need to satisfy in general the above boundary conditions. What it is true is that such boundary conditions define a dense set in $L^2(R)$, not the whole space.

APPENDIX 2: MATRIX ELEMENTS

In this appendix we will describe with a certain accuracy the way in which the matrix elements V_{ijkl} occurring in the computation of the ground state energy can be exactly computed and their asymptotic expansions in the limit of small filling ν.

A2.1: Exact computation

The matrix element we want to compute, which is the general one appearing in Appendix 3 as a contribution to the energy, has the form already anticipated in Chapter 2, formula (2.23):

$$V_{ijkl} = \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, \Psi_i^*(\underline{r}_1) \, \Psi_j(\underline{r}_1) \, \Psi_k^*(\underline{r}_2) \, \Psi_l(\underline{r}_2) \qquad (A2.1)$$

where the wave functions, not mutually orthogonal, are

$$\Psi_j(x,y) = \frac{(-1)^{j_1 j_2}}{\sqrt{2\pi}} \, e^{i/2(Y_j x - X_j y)} \, e^{-(\underline{r} - \underline{R}_j)^2/4}$$

With the following positions

$$q_1 = \frac{1}{2}(\underline{R}_i + \underline{R}_j); \quad q_2 = \frac{1}{2}(\underline{R}_k + \underline{R}_l); \qquad \Delta_1 = \underline{R}_j - \underline{R}_i \; ; \qquad \Delta_2 = \underline{R}_l - \underline{R}_k \; ;$$

$$A_1 = \frac{1}{2}(\underline{R}_i - \underline{R}_j)^2; \quad A_2 = \frac{1}{2}(\underline{R}_l - \underline{R}_k)^2$$

V_{ijkl} can be written in the form

$$V_{ijkl} = (-1)^{i_1 i_2 + j_1 j_2 + k_1 k_2 + l_1 l_2} \left(\frac{1}{2\pi}\right)^2 e^{-(A_1 + A_2)/4} \, I_{ijkl}$$

where

$$I_{ijkl} = \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, e^{-(\underline{r}_2 - \underline{q}_2)^2/2} \, e^{-(\underline{r}_1 - \underline{q}_1)^2/2} \, e^{i/2(\Delta_{1y}x_1 - \Delta_{1x}y_1 + \Delta_{2y}x_2 - \Delta_{2x}y_2)}$$

Let us now introduce the Fourier transform of the Coulomb potential in two dimensions. We have:

$$\frac{1}{|\underline{r}_1 - \underline{r}_2|} = \frac{1}{2\pi} \int \frac{d^2\underline{k}}{|\underline{k}|} \, e^{-i\underline{k}(\underline{r}_1 - \underline{r}_2)}$$

We define some new constants depending on the indexes:

$$\underline{\Theta}_1 = (\Delta_{1y}, -\Delta_{1x}); \quad \underline{\Theta}_2 = (\Delta_{2y}, -\Delta_{2x}) \qquad \Phi_1 = \exp\left\{\frac{i}{2}(\underline{q}_1 \cdot \underline{\Theta}_1 + \underline{q}_2 \cdot \underline{\Theta}_2)\right\}$$

and we change integration variables:

$$\underline{P}_1 = \frac{1}{\sqrt{2}}(\underline{r}_1 - \underline{q}_1); \qquad \underline{P}_2 = \frac{1}{\sqrt{2}}(\underline{r}_2 - \underline{q}_2)$$

Putting the above form of the Coulomb potential in I_{ijkl} and separating the variables in the integrals we get

$$I_{ijkl} = \frac{2}{\pi}\Phi_1 \int \frac{d^2\underline{k}}{|\underline{k}|} \, e^{-i\underline{k}\cdot(\underline{q}_1 - \underline{q}_2)} \int d^2\underline{P}_1 \, e^{i\sqrt{2}(\frac{1}{2}\underline{\Theta}_1 - \underline{k})\cdot\underline{P}_1} \, e^{-\underline{P}_1^2} \; .$$

$$\cdot \int d^2\underline{P}_2 \, e^{i\sqrt{2}(\frac{1}{2}\underline{\Theta}_2 + \underline{k})\cdot\underline{P}_2} \, e^{-\underline{P}_2^2}$$

The gaussian integrations can be easily performed since they do not present any difficulty. It is convenient to define more vectors in order to obtain a simple form of the remaining two-dimensional integral on $\underline{k}$. We introduce

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$$\underline{R}_o = \underline{q}_1 - \underline{q}_2; \qquad \underline{v} = \underline{\Theta}_1 - \underline{\Theta}_2; \qquad \underline{v}_c = \frac{1}{2}\underline{v} - i\,\underline{R}_o$$

so that, reassembling all the results, we get

$$V_{ijkl} = (-1)^{i_1 i_2 + j_1 j_2 + k_1 k_2 + l_1 l_2}\,\frac{\Phi_1}{2\pi}\,e^{-(A_1+A_2)/2}\,H_{ijkl}$$

H_{ijkl} being

$$H_{ijkl} = \int \frac{d^2\underline{k}}{|\underline{k}|}\,e^{\underline{k}\cdot\underline{v}_c}\,e^{-\underline{k}^2} = \int_0^{2\pi} d\theta \int_0^{\infty} dk\, e^{kv_c\cos\theta}\,e^{-\underline{k}^2}$$

The angular integral gives origin to a Bessel function. In fact the integral definition of the modified Bessel function I_0, see for example reference [26], is

$$2\pi\, I_0(z) = \int_0^{2\pi} d\theta\, e^{-z\cos\theta}$$

In the same reference is contained an integral that is relevant in order to compute H_{ijkl}:

$$\int_0^{\infty} dx\, e^{-\alpha x^2}\,I_\nu(\beta x) = \sqrt{\frac{\pi}{4\alpha}}\,\exp\left(\frac{\beta^2}{8\alpha}\right) I_{\nu/2}\left(\frac{\beta^2}{8\alpha}\right) \qquad (\text{Re } \alpha > 0,\ \text{Re } \nu > -1)$$

Using the above integral it is possible conclude that

$$V_{ijkl} = \vartheta_1 \sqrt{\frac{\pi}{4}}\,e^{-(A_1+A_2)/2}\,e^{\underline{v}_c^2/8}\,I_0(\underline{v}_c^2/8) \qquad (A2.2)$$

where, we recall:

$$\underline{q}_1 = \frac{1}{2}(\underline{R}_i + \underline{R}_j); \qquad \underline{q}_2 = \frac{1}{2}(\underline{R}_k + \underline{R}_l); \qquad \underline{R}_o = \underline{q}_1 - \underline{q}_2$$

$$\underline{\Delta}_1= \underline{R}_j - \underline{R}_i \; ; \quad \underline{\Delta}_2= \underline{R}_l - \underline{R}_k \; ; \quad \underline{\Theta}_1= (\Delta_{1y}, - \Delta_{1x}); \quad \underline{\Theta}_2= (\Delta_{2y}, - \Delta_{2x})$$

$$(A2.3)$$

$$A_1 = \frac{1}{2} (\underline{R}_i - \underline{R}_j)^2, \quad A_2 = \frac{1}{2} (\underline{R}_l - \underline{R}_k)^2; \quad \underline{v} = \underline{\Theta}_1 - \underline{\Theta}_2; \quad \underline{v}_c = \frac{1}{2} \underline{v} - i \, \underline{R}_o$$

$$\vartheta_1 = (-1)^{i_1 i_2 + j_1 j_2 + k_1 k_2 + l_1 l_2} \exp\left\{\frac{i}{2} (\underline{q}_1 \cdot \underline{\Theta}_1 + \underline{q}_2 \cdot \underline{\Theta}_2)\right\}$$

We observe that the above formula coincides with the results in [7] for particular choices of indexes.

A2.2: Asymptotic expansion

Here we discuss the form of (A2.2) in the limit of electron filling going to zero. We want to remind first that the filling v appears in the above formula through the vectors $\underline{R}_n$. In fact they contain the lattice constant a, and a is, as a matter of fact, a v-depending function, see for example formula (2.31). This implies that the limit of small v is equivalent to the limit of large arguments $\underline{v}_c^2/8$ of the Bessel function. We therefore use the asymptotic expansion already introduced in Chapter 2. For Re[z] $\rightarrow \infty$ we have:

$$I_0(z) \approx \frac{e^z}{\sqrt{2\pi z}} \left\{ \frac{\Gamma(1/2)}{\Gamma(1/2)} - \frac{1}{2z} \frac{\Gamma(3/2)}{\Gamma(-1/2)} + \frac{1}{4z2} \frac{\Gamma(5/2)}{2! \, \Gamma(-3/2)} + \cdots \right\}$$

which becomes, expliciting the values of the Gamma functions, and considering only the first two terms above,

$$I_0(z) \underset{\mathrm{Re}[z]\to\infty}{\approx} \frac{e^z}{\sqrt{2\pi z}} \left\{ 1 + \frac{1}{8z} \right\} \qquad (A2.4)$$

This expansion is valid for large positive arguments of the real part of z. If Re[z] < 0 then we take into account the parity property of I_0, that is $I_0(z) = I_0(- z)$. Therefore we can write

$$I_0(z) \approx_{\mathrm{Re}[z] \to -\infty} \frac{e^{-z}}{\sqrt{-2\pi z}} \left\{ 1 - \frac{1}{8z} \right\} \qquad (A2.5)$$

The two formulas above can be used now to expand (A2.2). The result is easily obtained:

- $\mathrm{Re}[\underline{v}_c^2] > 0$

$$V_{ijkl} = \vartheta_1 \; e^{-\frac{1}{4}[2(A_1+A_2)-\underline{v}_c^2]} \frac{1}{\sqrt{\underline{v}_c^2}} \left\{ 1 + \frac{1}{\underline{v}_c^2} \right\} \qquad (A2.6)$$

- $\mathrm{Re}[\underline{v}_c^2] < 0$

$$V_{ijkl} = \vartheta_1 \; e^{-\frac{1}{2}(A_1+A_2)} \frac{1}{\sqrt{-\underline{v}_c^2}} \left\{ 1 - \frac{1}{\underline{v}_c^2} \right\} \qquad (A2.7)$$

We see that there is a difference in the asymptotic behaviour depending on the sign of $\mathrm{Re}[\underline{v}_c^2]$. This implies that, to correctly estimating the orders of the various contributions coming out in our perturbation approach we need to compute first $\mathrm{Re}[\underline{v}_c^2]$ for any such contributions and then use (A2.6) or (A2.7).

Let us now discuss a crucial point of the above expansion: equation (A2.6) shows that a divergent behaviour of the matrix elements seems in principle to be allowed for some value of the indexes. This can actually be proven not to be the case. In fact studying the modulus of V_{ijkl} it is very easy to obtain the following estimate:

$$|V_{ijkl}| \le e^{-\frac{1}{4}(A_1+A_2)} \qquad (A2.8)$$

Here all the irrelevant constants have been neglected, since they do not modify the asymptotic behaviour, and A_1 and A_2 are defined in (A2.3). This is a crucial result since it ensure that all the matrix elements present in each term of the perturbative expansion, see the explicit form (A3.5), can only improve the net order of a single term (that is the power of its coefficient $\exp\{-R_{10}^2/4\}$), or leave it unchanged.

APPENDIX 3: ENERGY COMPUTATION

Here we will show in many details how to compute the correction δE in (2.21), starting with $E(N)/N$ for N going to infinity. In fact we already know the form of $\lim_{N\to\infty} E_w(N)/N$ that has to be subtracted to $\lim_{N\to\infty} E(N)/N$ to get δE. We therefore concentrate our attention on the computation of E_I in (2.22):

$$E_I = \lim_{N\to\infty} E(N)/N = \frac{1}{2} \sum_{i\neq 0} \left\{ E_d(i,0) - E_s(i,0) \right\} \qquad (A3.1)$$

where

$$E_d(i,0) = \int d^2\underline{r}_1 \, d^2\underline{r}_2 \, \frac{|\Omega_i(\underline{r}_1)|^2 \, |\Omega_0(\underline{r}_2)|^2}{|\underline{r}_1 - \underline{r}_2|} \qquad (A3.2)$$

and

$$E_s(i,0) = \int d^2\underline{r}_1 \, d^2\underline{r}_2 \, \frac{\Omega_i{}^*(\underline{r}_1) \, \Omega_0{}^*(\underline{r}_2) \, \Omega_0(\underline{r}_1) \, \Omega_i(\underline{r}_2)}{|\underline{r}_1 - \underline{r}_2|} \qquad (A3.3)$$

Using the form of the orthonormal state Ω_i given in (2.13)

$$\Omega_i \approx \Psi_i - \frac{1}{2} \sum_{n\neq 0} c_n \, \Psi_{i+n} + \frac{3}{8} \sum_{n} \sum_{s\neq 0 \, (s\neq n)} c_{n-s} \, c_s \Psi_{i+n} \qquad (A3.4)$$

and introducing the definition of the matrix elements V_{ijkl}, we can expand $E_d(i,0)$ and $E_s(i,0)$ in terms of the coefficients c_n. We stress that in this expansion we can neglect all the terms in which appear more than two coefficients c_n. In fact, due to the estimate at the end of Appendix 2, we are sure that the V_{ijkl} cannot be of the order $c_n{}^{-k}$, k being a positive integer. By their own nature the V_{ijkl} terms can only improve or leave unchanged the decay behaviour of the single terms. This implies that the contributions we start considering are, in effect, more than the ones we

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should consider in a correct counting of the net orders. This point will be analyzed in details for some of the contributions below, to clarify this problem and to insert all these points in a well defined scheme. In particular we will show how the terms of the net order bigger than c_{10}^2 are found and eliminated.

The direct and the exchange terms become respectively:

$$E_d(i,0) = V_{iioo} - \sum_n \left\{ c_{n\neq 0} - \frac{3}{4} \sum_{\substack{l\neq n \\ l\neq 0}} c_{n-1} c_l \right\} Re[V_{iion} + V_{ii+noo}] +$$

$$(A3.5)$$

$$+ \frac{1}{4} \sum_{\substack{l\neq 0 \ n\neq 0}} c_n c_l \, Re[V_{iiln} + V_{i+1\,i+noo}] + \frac{1}{2} \sum_{\substack{l\neq 0 \ n\neq 0}} c_n c_l \, Re[V_{ii+lon} + V_{ii+lno}]$$

$$E_s(i,0) = V_{iooi} - \sum_n \left\{ c_{n\neq 0} - \frac{3}{4} \sum_{\substack{l\neq n \\ l\neq 0}} c_{n-1} c_l \right\} Re[V_{ioni} + V_{i+nooi}] +$$

$$(A3.6)$$

$$+ \frac{1}{4} \sum_{\substack{l\neq 0 \ n\neq 0}} c_n c_l \, Re[V_{inli} + V_{i+nooi+l}] + \frac{1}{2} \sum_{\substack{l\neq 0 \ n\neq 0}} c_n c_l \, Re[V_{inoi+l} + V_{ioni+l}]$$

Some of these contributions are easy to compute. This is the case, for instance, of V_{iioo} and V_{iooi}. Using (A2.2) and (A2.3) one immediately gets:

$$V_{iioo} = \sqrt{\frac{\pi}{4}} \, e^{-R_i^2/8} \, I_0(R_i^2/8) \qquad \cdot$$

$$V_{iooi} = \sqrt{\frac{\pi}{4}} \, e^{-3R_i^2/8} \, I_0(R_i^2/8)$$

whose expansion can be obtained using the relevant expansion between (A2.6) and (A2.7). In order to decide which of the two formulas must be

used we compute first $\text{Re}[\underline{v}_c^2]$ for the above matrix elements. For V_{iioo} we obtain $\text{Re}[\underline{v}_c^2] = -\underline{R}_i^2 < 0$. We use therefore (A2.7) and we find

$$V_{iioo} = \frac{1}{|\underline{R}_i|}\left\{ 1 - \frac{1}{|\underline{R}_i|^2} \right\}$$

For what concerns V_{iooi} we obtain $\text{Re}[\underline{v}_c^2] = \underline{R}_i^2 > 0$ so that the correct expansion is the one in (A2.6). We therefore get:

$$V_{iooi} = e^{-\frac{1}{4}\underline{R}_i^2}\frac{1}{|\underline{R}_i|}\left\{ 1 + \frac{1}{|\underline{R}_i|^2} \right\}$$

Confronting these two behaviours we see that the exchange term contains in itself a damping exponential of the order $c_{1,0}$, see (1.18). This feature is an explicit example of what we discussed before, that is the natural improvement of the net perturbative order given by the matrix elements.

It is useful to consider almost all the details of the computation of a more involved term, for example in (A3.5). We consider

$$E_1 = \frac{3}{4}\sum_n \sum_{\substack{l\neq n \\ l\neq 0}}^{l\neq n} c_{n-l}\, c_l\, \text{Re}[\, V_{ii+noo}\,]$$

From (A2.3) we get:

$$\underline{q}_1 = \frac{1}{2}\underline{R}_n + \underline{R}_i\, ; \quad \underline{q}_2 = 0; \quad \underline{R}_o = \frac{1}{2}\underline{R}_n + \underline{R}_i; \quad \Delta_1 = \underline{R}_n\, ; \quad \Delta_2 = \underline{0}$$

$$\underline{\Theta}_1 = (Y_n, -X_n); \quad \underline{\Theta}_2 = 0; \quad A_1 = \frac{1}{2}\underline{R}_n^2; \quad A_2 = 0; \quad \underline{v} = (Y_n, -X_n)$$

$$\underline{v}_c^2 = -\underline{R}_i^2 - \underline{R}_i\cdot\underline{R}_n - i\,(\, X_i Y_n - X_n Y_i\,)$$

from where we see that $\text{Re}[\underline{v}_c^2]$ has not a definite sign, at least if i belongs to the first two shells. A deeper analysis is therefore required. From (A2.7) we see that, if $\text{Re}[\underline{v}_c^2] \leq 0$, then V_{ii+noo} goes like $\exp(-\underline{R}_n^2/4)$. Since this exponential must be multiplied for $c_{n-l}\, c_l$, $l\neq n$ and $l\neq 0$, we deduce that

only n=0 contributes in our scheme at the desired order. If, on the contrary, $\text{Re}[\underline{v}_c{}^2] > 0$, then (A2.6) provides the following behaviour: $V_{ii+noo} \approx \exp\{-(\underline{R}_n{}^2 + \underline{R}_i{}^2 + \underline{R}_i\cdot\underline{R}_n)/4\}$. In order to have a relevant contribution when multiplied for $c_{n-1}\, c_l$, we need to have, as before, the exponential equal to one, so that $\underline{R}_n{}^2 + \underline{R}_i{}^2 + \underline{R}_i\cdot\underline{R}_n = 0$. This equation must be satisfied together with the hypothesis $\text{Re}[\underline{v}_c{}^2] > 0$, that is $\underline{R}_i{}^2 + \underline{R}_i\cdot\underline{R}_n < 0$. It is easy to see that both conditions cannot be simultaneously solved, and therefore the only relevant contribution is the one with n=0 and $\text{Re}[\underline{v}_c{}^2] < 0$. We conclude that in our approximation it results

$$E_l = \frac{3}{4} \sum_{l \neq 0} c_l{}^2 \, \text{Re}[\, V_{iioo}\,]$$

and we have already computed V_{iioo} both in the exact and in the asymptotic form.

The other terms in (A3.5) and (A3.6) are all computed in analogous way: first one computes explicitly $\text{Re}[\underline{v}_c{}^2]$ for a given matrix element; then one considers the asymptotic behaviour of the product of such elements with the relative coefficients c_n. Only the terms of the summation up of the order $\exp(-\underline{R}_{10}{}^2/2)$, for the $v = 1/3$ lattice, are extracted from the various contributions, and finally these are computed and the exact or expanded results are given.

We give the final exact result E_I in (A3.1) without further comments:

$$E_I = \sqrt{\frac{\pi}{4}} \sum_{i \neq 0} \left\{ \frac{1}{2} e^{-\underline{R}_i{}^2/8} \, I_0(\underline{R}_i{}^2/8) + \frac{3}{4} \sum_{n \neq 0} c_n{}^2 \, e^{-\underline{R}_i{}^2/8} \, I_0(\underline{R}_i{}^2/8) \right. -$$

$$- \sum_{n \neq 0}^{(i \neq n)} c_n{}^2 \text{Re}\left[e^{\underline{R}_{in;c}{}^2/8} I_0(\underline{R}_{in,c}{}^2/8) \right] + \frac{1}{4} \sum_{n \neq 0}^{(i \neq n)} c_n{}^2 \, e^{-(\underline{R}_i - \underline{R}_n)^2/8} I_0((\underline{R}_i - \underline{R}_n)^2/8) -$$

$$\left. - \frac{1}{2} e^{-3\underline{R}_i{}^2/8} \, I_0(\underline{R}_i{}^2/8) - \frac{1}{4} c_i{}^2 \, e^{-\underline{R}_i{}^2/8} \, I_0(\underline{R}_i{}^2/8) \right\} \qquad \text{(A3.7)}$$

where we have defined the following complex quantity

$$\underline{R}_{in,c}{}^2 = -\underline{R}_i{}^2 + \underline{R}_i\cdot\underline{R}_n + i(X_i Y_n - X_n Y_i) \qquad \text{(A3.8)}$$

In view of a computer implementation we need to expand the Bessel function for large values of the arguments. Therefore (A3.7) will be used for computing the contributions coming from the first three 'shell' of the lattice around the origin while the other contributions must be computed using formula (A3.9) below.

$$E_I = \sum_{i \neq 0} \left\{ \frac{1}{2}\left[\frac{1}{|\underline{R}_i|} + \frac{1}{|\underline{R}_i|^3}\right] + \frac{3}{4}\sum_{n \neq 0} c_n^2 \left[\frac{1}{|\underline{R}_i|} + \frac{1}{|\underline{R}_i|^3}\right] - \right.$$

$$- \sum_{n \neq 0}^{(i \neq n)} c_n^2 \left[\frac{1}{|\underline{R}_{in;c}|} + \frac{1}{|\underline{R}_{in;c}|^3}\right] + \frac{1}{4}\sum_{n \neq 0}^{(i \neq n)} c_n^2 \left[\frac{1}{|\underline{R}_i - \underline{R}_n|} + \frac{1}{|\underline{R}_i - \underline{R}_n|^3}\right] -$$

$$\left. - \frac{1}{2} e^{-\underline{R}_i^2/4}\left[\frac{1}{|\underline{R}_i|} + \frac{1}{|\underline{R}_i|^3}\right] - \frac{1}{4} c_i^2 \left[\frac{1}{|\underline{R}_i|} + \frac{1}{|\underline{R}_i|^3}\right] \right\} \tag{A3.9}$$

We notice that the third contribution contains a square root of a complex quantity $\underline{R}_{in,c}$. Such root needs to be defined. To do it we start observing that, after subtracting the classical WC in (2.26), another divergence can still appear when the summation over i is performed: the second, the third and the fourth terms above are, in fact, one by one divergent due to the presence of an $1/|\underline{R}_i|$ term. However if we consider the sum of the three contributions it follows that, requiring the finiteness of the result, we univocally fix the definition of $|\underline{R}_{in,c}|$. To be explicit, the above condition forces us to define

$$Re\left[\frac{1}{|\underline{R}_{in;c}|}\right] = r_{in}^{-1/2} \cos(\theta_{in}/2)$$

where

$$r_{in} = |\underline{R}_{in,c}| = [(\underline{R}_i^2 - \underline{R}_i \cdot \underline{R}_n)^2 + (X_i Y_n - X_n Y_i)^2]^{1/2}$$

$$\theta_{in} = arctg\left\{\frac{X_n Y_i - X_i Y_n}{\underline{R}_i^2 - \underline{R}_i \cdot \underline{R}_n}\right\}$$

It is useful to notice here the practical relevance of the $(-1)^{nm}$ used in the definition of the original wave function. It is possible to see, but it is even a long and boring job, that, starting with a wave function without this phase factor, such a cancellation of divergences up to the second order, throughout being dictated by physical reasons, is not as much evident as it is with our definition. This is the main reason why we have keepen on using our definition.

We end this Appendix giving the asymptotic form of the correction δE to the ground state energy as it is obtained from (A3.9), (2.21), (2.22) and (2.26).

$$
\begin{aligned}
\delta E = \sum_{i \neq 0} \Bigg\{ & \frac{1}{2} \frac{1}{|R_i|^3} + \frac{3}{4} \sum_{n \neq 0} c_n{}^2 \left[\frac{1}{|R_i|} + \frac{1}{|R_i|^3} \right] + \frac{1}{4} \sum_{n \neq 0}^{(i \neq n)} c_n{}^2 \left[\frac{1}{|R_i - R_n|} + \frac{1}{|R_i - R_n|^3} \right] - \\
& - \sum_{n \neq 0}^{(i \neq n)} c_n{}^2 \left[\frac{1}{\sqrt{r_{in}}} \cos(\theta_{in}/2) + \frac{1}{\sqrt{r_{in}{}^3}} \cos(3\theta_{in}/2) \right] - \\
& - \frac{1}{2} e^{-R_i{}^2/4} \left[\frac{1}{|R_i|} + \frac{1}{|R_i|^3} \right] - \frac{1}{4} c_i{}^2 \left[\frac{1}{|R_i|} + \frac{1}{|R_i|^3} \right] \Bigg\}
\end{aligned}
$$

$$\text{(A3.10)}$$

APPENDIX 4: POLARIZATION CORRECTIONS

The starting point is the matrix elements in (4.12)

$$E'_d(i,0) = \int d^2\underline{r}_1 \, d^2\underline{r}_2 \, \frac{|\xi_i(\underline{r}_1)|^2 \, |\xi_0(\underline{r}_2)|^2}{|\underline{r}_1 - \underline{r}_2|} \qquad (A4.1)$$

where we recall that the functions $\xi_i(\underline{r}_1)$ are defined in (4.5) and (4.7):

$$\xi_0(z) = d_0 \, \Phi_0(z) + d_6 \, \Phi_6(z) \qquad (A4.2)$$

$$\xi_i(z) = (-1)^{i_1 i_2} \, e^{i/2(Y_i x - X_i y)} \, \xi_0(\underline{r} - \underline{R}_i) \qquad (A4.3)$$

Substituting the explicit form of the functions ξ_n in E'_d we get 16 terms, some of which are related each other. We need therefore to compute 6 contributions, all containing integrals of gaussian functions multiplied with a Coulomb factor. Being the original integrations absolutely convergent we can use some 'trick' to obtain a common expression for all of these. We write down only some of these integrals:

$$I_1 = \lim_{\alpha,\beta \to 1} (2\pi)^{-2} \, \alpha\beta \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, e^{-\alpha \underline{r}_2{}^2/2} \, e^{-\beta(\underline{r}_1 - \underline{R}_i)^2/2}$$

$$I_2 = \lim_{\alpha,\beta \to 1} (2\pi)^{-2} \, \frac{\beta\alpha^7}{6!} \, \frac{d^6}{d\alpha^6} \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, e^{-\alpha \underline{r}_2{}^2/2} \, e^{-\beta(\underline{r}_1 - \underline{R}_i)^2/2}$$

$$I_3 = \lim_{\alpha,\beta \to 1} (2\pi)^{-2} \, \frac{\beta^7\alpha^7}{(6!)^2} \, \frac{d^6}{d\alpha^6} \, \frac{d^6}{d\beta^6} \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, e^{-\alpha \underline{r}_2{}^2/2} \, e^{-\beta(\underline{r}_1 - \underline{R}_i)^2/2}$$

and so on. The general form at which all the integrals can be reconducted is the following one:

$$I = \int \frac{d^2\underline{r}_1 \, d^2\underline{r}_2}{|\underline{r}_1 - \underline{r}_2|} \, e^{-\alpha(\underline{r}_2 - \underline{R}_2)^2/2} \, e^{-\beta(\underline{r}_1 - \underline{R}_i)^2/2} \tag{A4.4}$$

whose computation follows exactly the same steps discussed in Appendix 2 for the 'standard' matrix elements. The exact result is

$$I = \frac{\pi^{5/2} 2^{3/2}}{\sqrt{\alpha\beta(\alpha+\beta)}} e^{-\frac{\alpha\beta}{4(\alpha+\beta)}|\underline{R}_i - \underline{R}_2|^2} \, I_0\left(\frac{\alpha\beta}{4(\alpha+\beta)}|\underline{R}_i - \underline{R}_2|^2\right) \tag{A4.5}$$

One of the main difficulty that comes out from the above formula is that we do not know how to compute high order derivatives of the I_0 Bessel function, which we have to know since they enter the definitions of I_2, I_3, and so on. Consequently, it is convenient to consider the asymptotic expansion of the above result, that is

$$I \approx \frac{(2\pi)^2}{\alpha\beta} \frac{1}{|\underline{R}_i - \underline{R}_2|} \left\{ 1 + \frac{1}{|\underline{R}_i - \underline{R}_2|^2} \frac{(\alpha+\beta)}{2\alpha\beta} \right\} \tag{A4.6}$$

Using this formula it is now straightforward to find the result in (4.15).

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