We introduce and study the Wannier functions for an electron moving in a plane under the influence of a perpendicular uniform and constant magnetic field. The relevance for the Fractional Quantum Hall Effect is discussed; in particular it shown that an interesting Hartree-Fock state can be constructed in terms of Wannier functions.

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I. INTRODUCTION

It is widely accepted that Quantum Hall Effect \([1,2]\) can be described by a model of interacting electrons moving in a plane. For many features of the phenomenon the zero temperature limit seems to be a good approximation.

In the attempt to describe the state in terms of single particle approximation and subsequent perturbations around this trial state, the author has introduced \([3]\) a set of functions which are eigenfunctions of the single particle Hamiltonian and moreover are invariant, up to a phase, under finite translations associated to a lattice. The phase depends on the coordinates. In subsequent papers \([4,5]\) an \textit{Ansatz} was introduced in order to construct the trial state. In Ref. \([5]\) numerical evidence is given that this state yields a mean Coulomb energy close to the value provided by genuine many-body states (e.g. Laughlin’s \([6]\)). From this property and from the fact that the trial state is given in analytic form in terms of a Slater determinant (or single particle approximation) the author hopes that a perturbative approach based on this \textit{Ansatz} will improve the value of the mean energy and provide a further progress in the understanding of the phenomenon.

In this note the Wannier functions are introduced by using the functions invariant under translations. This construction has some degree of arbitrariness related to the phase, which cannot be fixed \textit{a priori}. Some possible natural choices are considered and numerical methods are used in order to decide which is the better one.

Finally the Wannier functions are used in order to reformulate the \textit{Ansatz} for the trial state. This analysis shows that there is at least another natural candidate for the trial state. By considering the particular case of filling factor 1/3 numerical evidence is given that the original proposal gives the better choice.

II. THE FORMALISM

In this section some essential points developed in I and III are briefly reviewed. The Hamiltonian for the single electron is

\[
H = \frac{1}{2} \left[ \left( -i \partial_x - \frac{y}{2} \right)^2 + \left( -i \partial_y + \frac{x}{2} \right)^2 \right]
\]

where the unit of length is

\[
\lambda = \left( \frac{\hbar}{eB} \right)^{\frac{1}{2}}
\]

and the unit of energy

\[
\hbar \omega_c = \hbar \frac{eB}{mc}
\]

The complex notation is used for the vectors
\[ w = w_1 + i w_2. \]  

(4)

Step down and step operators are defined

\[
\begin{align*}
    a & \equiv \frac{1}{\sqrt{2}} \left( \frac{w^*}{2} + 2 \partial w \right) \\
    b & \equiv \frac{1}{\sqrt{2}} \left( \frac{w}{2} + 2 \partial w^* \right).
\end{align*}
\]

(5)

They obey the algebra

\[
\begin{align*}
[a, a^\dagger] &= 1 & [b, b^\dagger] &= 1 \\
[a, b^\dagger] &= 0 & [a, b] &= 0
\end{align*}
\]

(6)

and moreover

\[
H = a^\dagger a + \frac{1}{2}.
\]

(7)

Let \( \varphi_{n_L} \) be the solution of

\[
\begin{align*}
a^\dagger a \varphi_{n_L} &= n_L \varphi_{n_L} \\
b \varphi_{n_L} &= 0.
\end{align*}
\]

(8)

One gets easily

\[
\varphi_{n_L}(r) = (2\pi n_L!)^{-\frac{1}{2}} \left( \frac{x + iy}{\sqrt{2}} \right)^{n_L} \exp \left( -\frac{r^2}{4} \right).\]

(9)

It is convenient to introduce the coherent-state operator

\[
S(w) = \exp \left( \frac{1}{\sqrt{2}}(w^* b - wb^\dagger) \right) = \exp \left( \frac{i}{2} \mathbf{w} \times \mathbf{r} \cdot \mathbf{\hat{z}} \right) \exp \left( w_1 \partial_x + w_2 \partial_y \right)
\]

(10)

i.e. it is the product of a translation and a phase. It has the properties

\[
[S(w), H] = 0
\]

(11)

and

\[
S(c)S(d) = S(c + d) \exp \left( -\frac{i}{2} \mathbf{c} \times \mathbf{d} \cdot \mathbf{\hat{z}} \right)
\]

(12)

(Magnetic Translation Group (MTG)). Thus they commute

\[
[S(c), S(d)] = 0 \quad \text{if} \quad \mathbf{c} \times \mathbf{d} \cdot \mathbf{\hat{z}} = 2\pi u \quad (u \text{ integer}).
\]

(13)

Then these operators are adequate in order to impose quasi-periodic boundary conditions on a parallelogram \( A \) with side vectors \( \mathbf{L}_1, \mathbf{L}_2 \)

\[
\begin{align*}
S(\mathbf{L}_1) \psi &= e^{i \theta_1} \psi \\
S(\mathbf{L}_2) \psi &= e^{i \theta_2} \psi
\end{align*}
\]

(14)

provided they commute

\[
[S(\mathbf{L}_1), S(\mathbf{L}_2)] = 0 \quad \text{i.e.} \quad \mathbf{L}_1 \times \mathbf{L}_2 \cdot \mathbf{\hat{z}} = 2\pi g_L \quad (g_L \text{ integer}).
\]

(15)

Then \( g_L \) will be the degeneracy of the Landau levels. The elements of the MTG are defined by the constraint

\[
[S(w), S(L_j)] = 0 \quad j = 1, 2
\]

(16)

i.e.
\[ w = \frac{1}{g_L}(-n_1 L_2 + n_2 L_1) \quad \text{with} \quad n_1, n_2 \text{ integers.} \] (17)

Let \( c, d \) be any two vectors that satisfy eq. (13) and provide a commensurate tiling of the parallelogram, i.e.

\[
\begin{align*}
L_1 &= pc \\
L_2 &= p'c + qd
\end{align*}
\] (18)

where the coefficients are integers. One has

\[ g_L = pqu. \] (19)

A finer lattice can be introduced generated by the vectors \( f \) and \( g \) such that

\[
\begin{align*}
c &= \kappa f + \iota' g \\
d &= \kappa' f + \iota g
\end{align*}
\] (20)

with the condition that the coefficients are integer numbers and moreover

\[ f \times g \cdot \hat{z} = 2\pi \] (21)

i.e.

\[ \kappa L - \kappa' L' = u. \] (22)

Sets of functions can be introduced which are eigenvectors of the Hamiltonian and are invariant under translations given by the sites of the lattice generated by \( c, d \) or by \( f, g \). Thus solutions of

\[
S(c)\psi_{nL}^{\mu\nu}(r) = e^{i\mu}\psi_{nL}^{\mu\nu}(r)
\]

and

\[
S(d)\psi_{nL}^{\mu\nu}(r) = e^{i\nu}\psi_{nL}^{\mu\nu}(r)
\] (23)

and

\[
S(f)\phi_{nL}^{\alpha\beta}(r) = e^{i\alpha}\phi_{nL}^{\alpha\beta}(r)
\]

and

\[
S(g)\phi_{nL}^{\alpha\beta}(r) = e^{i\beta}\phi_{nL}^{\alpha\beta}(r)
\] (24)

can be introduced. The solutions of the above equations are given by

\[
\psi_{nL}^{\mu\nu}(r) = \left( pq \right)^{-\frac{1}{2}} \sum_{m,n=-\infty}^{+\infty} \left[ S(c) e^{-i\mu} \right]^m \left[ S(d) e^{-i\nu} \right]^n \varphi_{nL}(r)
\]

\[
= \left( pq \right)^{-\frac{1}{2}} \sum_{m,n=-\infty}^{+\infty} (-)^{mn} u \exp[-i(\mu m + \nu n)]
\]

\[
\exp \left[ \frac{i}{2} \hat{z} \cdot (mc + nd) \times r \right] \varphi_{nL}(r + mc + nd)
\] (25)

and similarly

\[
\phi_{nL}^{\alpha\beta}(r) = \left( g_L \right)^{-\frac{1}{2}} \sum_{m,n=-\infty}^{+\infty} \left[ S(f) e^{-i\alpha} \right]^m \left[ S(g) e^{-i\beta} \right]^n \varphi_{nL}(r)
\]

\[
= \left( g_L \right)^{-\frac{1}{2}} \sum_{m,n=-\infty}^{+\infty} (-)^{mn} \exp[-i(m\alpha + n\beta)]
\]

\[
\exp \left[ \frac{i}{2} \hat{z} \cdot (mf + ng) \times r \right] \varphi_{nL}(r + mf + ng).
\] (26)

The value of the parameters are fixed by the boundary conditions in eq. (14). See eqs. (49), (83) and (84) of I. In particular it is easy to find the following relations as a consistency condition for the eqs. (23) and (24).
\[ 2\pi n_1 + \mu = \pi \kappa' + \kappa + \ell' \beta \]
\[ 2\pi n_2 + \nu = \pi \kappa' + \kappa' \alpha + \i' \beta. \]  

(27)

The norm of the wave function is (see eqs. (69) and (91) of I)

\[ \| \phi^{\alpha\beta}_{n_L} \|^2 = \sum_{m,n=-\infty}^{+\infty} \int_{\mathbb{R}^2} d^2 r \{ [S(f)]^m [S(g)]^n \varphi_{n_L}^m (r) \}^* \varphi_{n_L}^n (r) e^{i(m \alpha + n \beta)}. \]  

(28)

One gets

\[ \| \phi^{\alpha\beta}_{n_L} \|^2 = \sum_{m,n=-\infty}^{+\infty} (-)^{mn} e^{i(m \alpha + n \beta)} \exp\left(-\frac{1}{4} |mf + ng|^2 \right). \]  

(29)

A similar result is valid for the other set of functions

\[ \| \psi^{\mu\nu}_{n_L} \|^2 = \sum_{m,n=-\infty}^{+\infty} (-)^{mn} e^{i(m \mu + n \nu)} \exp\left(-\frac{1}{4} |mc + nd|^2 \right). \]  

(30)

The set of functions \( \{ \phi^{\alpha\beta}_{n_L} \} \) form a complete set. We use capital letters to denote the normalized functions

\[ \Phi^{\alpha\beta} = \frac{\phi^{\alpha\beta}_{n_L}}{\| \phi^{\alpha\beta}_{n_L} \|} \]
\[ \Psi^{\mu\nu} = \frac{\psi^{\mu\nu}_{n_L}}{\| \psi^{\mu\nu}_{n_L} \|}. \]  

(31)

For computation of the matrix elements of the Coulomb part (in II and III) it was convenient to introduce a new set of functions \( \{ \hat{\phi}^{\alpha\beta}_{n_L} \} \). One considers a reference wave function \( \Phi^{\alpha\beta} \) and defines (see Appendix in III)

\[ \hat{\phi}^{\alpha\beta}_{n_L} \equiv S(w_{\alpha\beta}) \Phi^{\alpha\beta}_{n_L} \]  

(32)

where \( w_{\alpha\beta} \) is a standard set of vectors

\[ w_{\alpha\beta} = (2\pi)^{-1} \left[ (\beta - \beta_0) f - (\alpha - \alpha_0) g \right]. \]  

(33)

By using the composition rules in eq. (12)

\[ S(w_{\alpha\beta})S(f)S(w_{\alpha\beta}) \exp(-i w_{\alpha\beta} \times f \cdot \hat{z}) = S(f)S(w_{\alpha\beta}) \exp(-i(\alpha - \alpha_0)) \]
\[ S(w_{\alpha\beta})S(g)S(w_{\alpha\beta}) \exp(-i w_{\alpha\beta} \times g \cdot \hat{z}) = S(g)S(w_{\alpha\beta}) \exp(-i(\beta - \beta_0)) \]  

(34)

it is easy to show that \( \hat{\phi}^{\alpha\beta}_{n_L} \) satisfies eqs. (24) and therefore differs from \( \Phi^{\alpha\beta}_{n_L} \) by a phase.

III. WANNIER FUNCTIONS

In this section Wannier functions \( \mathcal{W}_{r,s} \) are introduced for a particle moving in a constant and homogeneous magnetic field. Various sets of Wannier functions can be introduced. By starting from \( \{ \Phi^{\alpha\beta}_{n_L} \} \) one can define (the index \( n_L \) will be suppressed for convenience of notation)

\[ \mathcal{W}_{r,s} \equiv g_L^{-\frac{1}{2}} \sum_{\alpha\beta} e^{-i(r \alpha + s \beta)} \hat{\phi}^{\alpha\beta}. \]  

(35)

If one uses the set \( \{ \hat{\phi}^{\alpha\beta}_{n_L} \} \) a different Wannier functions is obtained

\[ \hat{\mathcal{W}}_{r,s} \equiv g_L^{-\frac{1}{2}} \sum_{\alpha\beta} e^{-i(r \alpha + s \beta)} \hat{\phi}^{\alpha\beta}. \]  

(36)
Yet another Wannier function is obtained if $\hat{\Phi}_{nL}^{\alpha\beta}$ is replaced by
\begin{equation}
S(w_{\alpha_0\beta_0})S(w_{\alpha\beta})\Phi_{nL}^{\alpha\beta_0} = \exp\left(\frac{i}{4\pi}(\alpha - \alpha_0)(\beta - \beta_0)\right)\Phi_{nL}^{\alpha\beta}.
\end{equation}

All these definitions provide a set of orthonormal functions located around the lattice site
\begin{equation}
x = rf + sg.
\end{equation}
Moreover they have the property (see eq. (24))
\begin{equation}
S(x')W_{r,s}(x) = \exp\left(i2(r'f + s'g) \cdot \hat{z}\right)W_{r,s}(x + r'f + s'g)
= (-)^{r's'}W_{(r-r'),(s-s')}(x).
\end{equation}

One expects that any different choice of phases for the translation invariant functions provides Wannier functions with different shapes [9]. By numerical inspection one can chose the functions with better localization properties among the three proposal given in eqs. (35), (36) and (37). From Figs. 1, 2 and 3 one sees clearly that the choice in eq. (35) ($W_r^u$) gives the best localization.

The formalism developed in section II allows the introduction of other kind of Wannier functions, i.e. those associated to the lattice generated by the $c,d$ vectors [17].

\begin{equation}
W_{m,n}^{(u)}(x) = \left(\frac{u}{gL}\right)^{\frac{1}{2}} \sum_{\mu\nu} e^{-i(m\mu + n\nu)} \Phi_{\mu\nu}^{\alpha\beta}
\end{equation}
is expected to be localized around the lattice site
\begin{equation}
x = mc + nd.
\end{equation}

Fig. 4 shows the shape of the Wannier function $W_{m,n}^{(u)}$. It should be noticed that the functions $\{W_{m,n}^{(u)}\}$ do not form a complete set of functions.

It is interesting to elaborate further the difference between the sets $\{W\}$ and $\{W^{(u)}\}$. It can be shown (see eq. (90) of I) that
\begin{equation}
\psi_{nL}^{\mu\nu} = u^{-\frac{1}{2}} \sum_{\alpha\beta} \Phi_{nL}^{\alpha\beta}.
\end{equation}
On the other side, $\{W_{r,s}\}$ evaluated on a $c,d$ lattice site
\begin{align*}
r &= m\kappa + n\kappa' \\
s &= m\iota' + n\iota,
\end{align*}
gives (see eq. (27))
\begin{align*}
r\alpha + s\beta &= m(\kappa\alpha + \iota'\beta) + n(\kappa'\alpha + \iota\beta) \\
&= m[\mu - \pi\kappa\iota' + 2\pi n_1] + n[\nu - \pi\kappa'\iota + 2\pi n_2]
\end{align*}
and therefore
\begin{equation}
W_{r,s} = \exp(-i\pi(m\kappa\iota' + n\kappa'\iota)) \left(\frac{u}{gL}\right)^{\frac{1}{2}} \sum_{\mu\nu} e^{-i(m\mu + n\nu)} \left\{u^{-\frac{1}{2}} \sum_{\alpha\beta} \Phi_{nL}^{\alpha\beta}\right\}
\end{equation}
on the sites of the $c,d$ lattice.

The conclusion of this section is that one has two good candidates ($\{W_{r,s}\}$ and $\{W_{m,n}^{(u)}\}$) which can be used for the construction of a trial state for the many-body problem.
IV. TRIAL STATE FOR FQHE

The original Ansatz for the FQHE trial state presented in the papers II and III was formulated in terms of the wave function $\Psi_{\mu\nu}$ of eqs. (25) and (31). For the filling factor $1/u$ it is just the Slater determinant of the $g_L/u$ functions with $n_L = 0$. In the second quantization formalism where $\psi$ is fermion field (spin is neglected), the trial state is

$$|\Omega\rangle = \prod_{\mu\nu} \int_A d^2x \psi^\dagger(x) \Psi_{\mu\nu}(x) |0\rangle.$$  \hfill (46)

The equation (40) is a unitary transformation, thus, up to a phase, the state $|\Omega\rangle$ can be written in terms of Wannier functions

$$|\Omega\rangle \simeq \prod_{m,n} \int_A d^2x \psi^\dagger(x) W_{m,n}(x) |0\rangle,$$  \hfill (47)

where $m, n$ are the sites of the lattice generated by $c, d$.

From the discussion at the end of section III it follows that one can similarly construct a trial state in terms of the Wannier functions $W_{r,s}$ given in eq. (35)

$$|\tilde{\Omega}\rangle \equiv \prod_{m,n} \int_A d^2x \psi^\dagger(x) W_{r,s}(x) |0\rangle \left|\begin{array}{c} r = m_\kappa + n_\kappa' \\ s = m_\iota' + n_\iota \end{array}\right.$$

Both Ansätze have as rationale the strategy of placing the $N = g_L/u$ electrons on a regular lattice. Moreover a peaked distribution of the electron density around the sites diminishes the energy coming from the Coulomb repulsion.

Before examining the numerical consequences of the choices made in eqs. (47) and (48), it is interesting to look closer at the states occupied by the single electrons. In the state $|\Omega\rangle$ the electron with $\mu\nu$ quantum numbers is in a state given by (see eq. (42))

$$\psi_{\mu\nu} = u^{-\frac{1}{2}} \sum_{\alpha\beta} \phi_{\alpha\beta} = u^{-\frac{1}{2}} \sum_{\alpha\beta} ||\phi_{\alpha\beta}|| \Phi_{\alpha\beta},$$

while in the state $|\tilde{\Omega}\rangle$ (see eq. (47)) is described by the wave function

$$u^{-\frac{1}{2}} \sum_{\alpha\beta} \Phi_{\alpha\beta}.$$  \hfill (50)

Thus in the first case the probability amplitude for the state $\Phi_{\alpha\beta}$ is proportional to $||\phi_{\alpha\beta}||$ and in the second is equal for all $\alpha\beta$ (fixed $\mu\nu$).

The two Ansätze given in eqs. (47) and (48) can be tested in the self-consistent equation based on the Hartree-Fock approximation (see eq. (158) of III). Fig. 5 shows that the state $|\Omega\rangle$ given in eq. (47) yields a better trial state (to a good approximation, it is unchanged by the self-consistent procedure).

1. K. von Klitzing, G. Dorda and M. Pepper, Phys. Rev. Lett. 45, 494 (1980).
2. D.C. Tsui, H.L. Störmer and A.C. Gossard, Phys. Rev. Lett. 48, 1559 (1982).
3. R. Ferrari, Phys. Rev. B42, 4598 (1990). This paper will be quoted as I.
4. R. Ferrari, Int. J. Mod. Phys. B 6, 2253 (1992). This paper will be quoted as II.
5. R. Ferrari, Int. J. Mod. Phys. B 8, 529 (1994). This paper will be quoted as III.
6. R.B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983). See also The Quantum Hall Effect edited by R.E. Prange and S.M. Girvin (Springer–Verlag, Berlin, 1990) 2nd ed.
7. J. Zak, Phys. Rev. 134, A1602 and A1607 (1964).
8. G.H. Wannier, Phys. Rev. 52, 191 (1937).
FIG. 1. 3D plot of the modulus of a Wannier function $W$ given in eq. (35). The lattice is regular and triangular ($|f| = |g| \sim 2.69$ in units of magnetic length). This picture is a zoom in on a domain whose size appears in Figs. 2 and 3.

FIG. 2. 3D plot of the modulus of a Wannier function $\hat{W}$ given in eq. (36). See Fig. 1 for details.

FIG. 3. 3D plot of the modulus of a Wannier function obtained by using the representation of the MTG given by the functions in eq. (37). See Fig. 1 for details.

FIG. 4. 3D plot of the modulus of a Wannier function $W^{(u)}$ given in eq. (40) ($\{c,d\}$ lattice, regular and triangular. $u = 3$ and therefore $|c| = |d| \sim 4.66$). This picture is a zoom in on the domain of definition, whose size appears in Figs. 2 and 3.

FIG. 5. Convergence patterns in the iteration procedure based on the self-consistent equation in the Hartree-Fock approximation. "Times" refer to the Ansatz based on the functions $W^{(u)}$ (eq. (47)) and "circles" to the Ansatz based on the functions $W$ (eq. (48)). Filling factor is $1/3$. 

9 W. Kohn, Phys. Rev. 115, 809 (1959).
10 G.H. Wannier, Rev. Mod. Phys. 34, 645 (1962).
11 E.I. Blount, Solid State Phys. 13, 305 (1962).
12 J. Des Cloizeaux, Phys. Rev. 129, 554 (1963).
13 J. Des Cloizeaux, Phys. Rev. 135, A685 (1964).
14 J. Des Cloizeaux, Phys. Rev. 135, A698 (1964).
15 A. Nenciu and G. Nenciu, Phys. Rev. B47, 10112 (1993).
16 M.R. Geller and W. Kohn, Phys. Rev. B 48, 14085 (1993). In this paper the main developments on Wannie r functions are reviewed.
17 R.A. Evarestov and V.P. Smirnov, Phys. Status Solidi B 180, 411 (1993).
Fig. 4
Fig. 5