Ground State of the Fermi Gas in 2D Lattices with a Magnetic Field: New Exact Results

1990 Europhys. Lett. 13 205

(http://iopscience.iop.org/0295-5075/13/3/003)

EUROPHYSICS LETTERS 1 October 1990

Europhys. Lett., 13 (3), pp. 205-210 (1990)

Ground State of the Fermi Gas in 2D Lattices with a Magnetic Field: New Exact Results.

R. RAMMAL (*) (§) and J. BELLISSARD (**)

(*) *Centre de Physique Théorique* (§§), *CNRS-Luminy*
Case 907, F-13288 Marseille Cedex 09, France
(**) *Université de Provence, Marseille*

(received 21 May 1990; accepted in final form 25 July 1990)

PACS. 03.65S – Semiclassical theories and applications.
PACS. 05.30F – Fermion systems and electron gas.
PACS. 72.15 – Electron conduction in metals and alloys.

Abstract. – The ground-state energy $E(\phi, \nu)$ of spinless noninteracting fermions in two-dimensional crystal lattices is studied as a function of the particle density ν and the magnetic flux ϕ. Using a semi-classical quantization method, $E(\phi, \nu)$ is calculated and shown to have an absolute minimum which corresponds to one flux quantum per particle. Explicit cusplike behaviour of $E(\phi, \nu)$ at fixed ν is found on a dense set of ϕ values and the analyticity of the ground-state energy in ν is precised.

The motion of an electron in a crystal lattice in the presence of an external magnetic field is one of the classical problems in solid-state physics. Recently there has been a renewal of interest on this subject because of its importance in various 2D physical interesting problems: quantized Hall effect [1], Anyon superconductivity [2], flux state model for high-temperature superconductivity [3], quasi-1D conductors, etc. Already, the spectrum of tight-binding electrons on a 2D lattice in a magnetic field has an extremely rich structure. The generic feature of this single-particle spectrum (self-similarity, nesting properties, gap labelling, etc.) are well studied [4, 5] for various 2D lattices.

Very recently [6], the search for a possible failure of the Fermi-liquid theory for high-T_c superconductors was at the origin of a new piece of physics for the Landau levels (LL) of Bloch electrons.

One of the consequences of the convoluted structure of the spectrum is the stabilization of the Fermi sea by the gaps which appears at every rational flux ϕ. Indeed, Anderson [3, 6] was probably the first to realize the possibility of an optimal flux corresponding to one quantum flux per particle. More precisely, for a given particle density ν of fermions, the

---

(§) Permanent address: Centre de Recherches sur les Très Basses Températures, CNRS, BP 166X, 25, av. des Martyrs, F-38042 Grenoble Cedex, France.

(§§) Laboratoire Propre, Centre National de la Recherche Scientifique.

actual ground state is achieved for $\phi = \nu$. This relation is at the heart of the Anyon superconductivity [2] (where it is called the fundamental relation). Since then, this conjecture has received a strong numerical support from various authors and for different lattice structures [7, 8]. Furthermore, the plot of the total energy at fixed ν exhibits clearly a cusplike structure with an absolute minimum at $\phi = \nu$ [8]. The complete absence of analytical or rigorous results for this very important conjecture motivated the work presented here.

In this letter, we report upon a summary of our results for this problem. The method we used is a semi-classical approach for Bloch electrons in a magnetic field [9]. Within the same algebraic framework, we were able to investigate the zero-field limit as well as the case of an arbitrary rational flux. A complete account of this systematic approach will be published elsewhere [10].

1. Low flux limit.

Let us consider the case of a 2D square lattice with lattice spacing a in a magnetic field H. The Hamiltonian of free fermions is given by $\mathscr{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j \exp[i\phi_{ij}] + \text{h.c.}$, where $\langle ij \rangle$ refers to nearest-neighbour sites and $\phi_{ij} = (2\pi/\phi_0) \int_i^j \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{l}$. In Landau's gauge $\boldsymbol{A} = (0, Hx)$ one obtains the eigenvalue equation

$$\psi(x+a, y) + \psi(x-a, y) + \exp[i\gamma x/a]\psi(x, y+a) + \exp[-i\gamma x/a]\psi(x, y-a) = (\varepsilon/t)\psi(x, y). \quad (1)$$

In eq. (1), $\gamma = 2\pi\phi/\phi_0$ and $\phi = Ha^2$ is the flux through the elementary cell, whereas ϕ_0 is the flux quantum. For the sake of simplicity, we will assume $\phi_0 = 1$ and $a = 1$. Assuming plane waves in the y-direction, $\psi(x, y) = \exp[ik_y y]\phi(j)$, $x = ja$, eq. (1) reduces to a 1D form known as Harper's equation:

$$\phi(j+1) + \phi(j-1) + 2\cos(\gamma j + k_y)\phi(j) = (\varepsilon/t)\phi(j). \quad (2)$$

Near the lowest band-edge of the zero-field limit, $\varepsilon(k_x, k_y) = -2t(\cos k_x + \cos k_y)$ and one recorvers, at first order in γ, the known free fermions LL: $\varepsilon_n/t = -4 + (2n+1)\gamma$ $(n \geqslant 0)$. One way to get this result is to use γj as a continuous variable and expanding both the difference and the potential terms in eq. (2). For a finite particle density ν and a given flux ϕ, the ground-state energy corresponding to a complete filling of a finite number of LL is known to be the same whatever the number of filled LL. The cause of this behaviour is the interplay between the energy ε_n and the degeneracy of each LL. Lifting this «degeneracy» of $E(\phi, \nu)$ by the lattice potential is therefore a highly nontrivial problem (singular perturbation). We found that a semi-classical approach is an appropriate tool for the asymptotic expansion of ε_n to an arbitrary order in γ. The method, which for $\gamma \approx 0$ is equivalent to the so-called Peierls substitution [9], can be outlined as follows. Expand the dispersion relation $\varepsilon(k_x, k_y)$ near the bottom of the band at $\gamma = 0$ and then substitute k_x by $\gamma^{1/2}K_1$ and k_y by $\gamma^{1/2}K_2$. Here K_1 and K_2 are magnetic translation operators with $[K_1, K_2] = i$. In the present case one gets the following Hamiltonian:

$$\mathscr{H}/t = -4 + \gamma(K_1^2 + K_2^2) - \gamma^2(K_1^4 + K_2^4)/12 + O(\gamma^3). \quad (3)$$

The first-order term in eq. (3) describes a simple harmonic oscillator, whereas the second

term is a perturbation. The final result is

$$\varepsilon_n/t = -4 + (2n+1)\gamma - \{(2n+1)^2+1\}\gamma^2/16 + O(\gamma^3), \qquad n \geqslant 0, \tag{4}$$

with the multiplicity $D = (H \cdot \text{Area})/\phi_0$.

Consider now N fermions on a lattice of N_s sites, so that $\nu = N/N_s$, and N_p plaquettes. It turns out that the appropriate variable to be considered is the ratio (called the filling factor) $x = N/D = (N_s/N_p)\,\nu/\phi$. Using a standard argument [11], the total energy is given by (n is fixed here by the filling factor x)

$$E = D\sum_{r=0}^{n-1}\varepsilon_r + (N - nD)\,\varepsilon_n, \qquad n \leqslant x < n+1. \tag{5}$$

Taking $\varepsilon(0) = -4t$ as the origin of energies, one obtains

$$2\frac{E}{N\zeta_0} = \frac{1}{x}\left\{(2n+1) - n(n+1)\frac{1}{x}\right\} - \frac{2}{x\zeta_0\Delta}\left(\frac{\zeta_0}{x}\right)^2 \cdot \left\{x\{(2n+1)^2+1\} - \frac{4}{3}n(n+1)(2n+1)\right\}, \qquad n \leqslant x < n+1, \tag{6}$$

where ζ_0 is the chemical potential at zero field and $\Delta = 64t$. The second term in eq. (6) comes from the lattice contribution, whereas the first one is the standard Fermi sea energy in the continuum. In the absence of the lattice term, E assumes the same minimum value at an infinite number of different filling factors: $x = 1, 2, 3, \ldots$ corresponding to cusps. The cusps are symmetric and each minimum describes a state with the n-lowest levels completely filled the others being empty. Now, if the second term in eq. (6) is included, the following properties hold:

i) the equality of the ground-state energy at different values of x is lifted out: the state corresponding to $x = 1$, is selected as the absolute minimum of E, whereas at $x = n$ one gets $2E/N\zeta_0 = 1 - (2 + 1/n^2)\,4\zeta_0/3\Delta$, and local cusplike minima appear at $x = 2, 3, \ldots$ etc.;

ii) the symmetry of the cusp of E *vs.* ϕ at $x = n$ is preserved for $1/N_s \cdot \partial E^{\pm}/\partial\phi = \pm\,\zeta_0/2 \cdot (1 - 8\zeta_0/\Delta)$ independently of n.

Result i) provides a perturbative proof for the conjecture $\nu = \phi$. Two questions arise from this finding: how general is the behaviour of $E(\phi, \nu)$ found here for the square lattice? Is result i) stable when further terms in eq. (4) are included? The first question is simply answered by the following generalization of eq. (4) to arbitrary periodic lattice:

Proposition 1. Suppose that near its minimum, $\varepsilon(k_x, k_y)$ assume the Taylor expansion in $\boldsymbol{k} = (k_x, k_y)$, $\varepsilon(k_x, k_y) = \varepsilon(0) + \omega(k_x^2 + k_y^2)/2 + O(|\boldsymbol{k}|^3)$ (where $\omega > 0$).

Then for $\gamma \approx 0$

$$\varepsilon_n = \varepsilon(0) + \frac{\omega\gamma}{2}(2n+1) + \frac{\gamma^2}{64}\Delta^2\varepsilon(0)\{(2n+1)^2+1\} - \ldots \ldots - \frac{\gamma^2}{288\omega}\{9(3n^2+3n+1)|\Delta\,\partial\varepsilon(0)|^2 + (3n^2+3n+2)|\partial^3\varepsilon(0)|^2\} + O(\gamma^3), \tag{7}$$

where $\partial = \partial/\partial k_x - i\,\partial/\partial k_y$ and $\Delta = \partial^2/\partial k_x^2 + \partial^2/\partial k_y^2$. ◇

If the lattice admits an inversion centre, namely if $\varepsilon(k_x, k_y) = \varepsilon(-k_x, -k_y)$, the last term in eq. (7) vanishes and one is reduced to the previous case, with a possible modification of ω and $\Delta^2\varepsilon(0)$. Therefore for usual lattice structures (square, triangular, honeycomb, generalized square, etc.), the absolute minimum of the ground-state energy is reached for $x = 1$, namely for $\phi = \nu N_s/N_p$. This results holds in general, provided the second-order term has the correct sign. Remark that the Hamiltonian need not admit only nearest-neighbours interaction to satisfy this result. The geometrical factor N_s/N_p assumes the values 1, 1/2, and 2 for square, triangular and honeycomb lattices, respectively, and the numerical finding of ref. [7] is recovered. In order to answer the second question, we have performed the next-order calculation of ε_n. A new term appears in eq. (4) which can be written as $\gamma^3\{n^3 + (n+1)^3\}/192$. In particular, for $x = n$ one gets the following expression for the energy per fermion (incorporating $\varepsilon(0) = -4$):

$$E/tN_s = -4\nu + 2\pi\nu^2 - \pi^2\nu^3/3 + \pi^3\nu^4/48 - \pi^2\nu^3/6n^2(1 - \pi\nu/8) \ldots . \tag{8}$$

Here again the absolute minimum is realized for $n = 1$ (compare with [8]). Similarly, the cusplike behaviour is preserved. However at this order in γ, the symmetry of the cusps is broken. Indeed the slopes are given by

$$1/N_s \cdot \partial E^{\pm}/\partial\phi = \pm\,\zeta_0/2 \cdot \{1 - 8\zeta_0/\Delta + 2\zeta_0^2/n^2\Delta' \cdot (3n^2 \pm n + 1)\}, \tag{9}$$

where $\Delta = 64t$, $\Delta'/\Delta = 24t$. In addition to the asymmetry of the cusp, an explicit dependence upon n takes place in eq. (9).

2. Arbitrary fluxes.

The previous result should actually apply to an arbitrary flux as long as the gap separating the LL does not close. Starting from the limit $\gamma \approx 0$, a periodic potential splits the LL into subbands and this results in broadening and a very intricated rich spectrum. The situation becomes simpler at rational fluxes $\phi = p/q$, where q subbands appear in the spectrum [4]. Then each subband has the same spectral weight $1/q$. For instance if $\nu = 1/q$, only the first subband is filled. Unless accidental degeneracy, the q subbands are separated by $q - 1$ gaps and within each gap the integrated density of states (IDS) is given by $r \cdot \phi + s$, where r, s are integers labelling the various gaps in the spectrum [4]. The couple $r = 1$, $s = 0$, corresponds to the main gap where the IDS is exactly equal to ϕ.

The stabilization of the Fermi sea at $\phi = \nu$ can be seen as follows, even though this is not yet supported by a rigorous proof. Let us start with simple LL, each having the degeneracy D. For N fermions, if the flux assumes the value ϕ_n such that $nD = N$, the ground state of the system will have the n-lowest levels completely filled, whereas the others will be empty. For our purpose, it is important to realize that whenever $\phi = \phi_n$, the ground state is isolated and separated from the first excited state by a finite gap equal to the gap between the n-th and the $(n+1)$-th LL of the one-particle Hamiltonian. At $\phi \neq \phi_n$, when the highest occupied single-particle level is not completely filled, the ground state is degenerate and is not separated by a gap from the excitation spectrum.

Assume now $\phi = \phi_n$ for some n, and let us turn on the interaction with the periodic potential of the lattice. As long as the gap between LL survives, the ground state remains nondegenerate and isolated from the rest of the spectrum. Having established that the ground state corresponds to $n = 1$ for low fields, this result remains valid for arbitrary values of the flux. Our argument is mainly based upon the continuity of the one-particle

spectrum with respect to ϕ and the strength of the interaction. This simply means that if the gap at $x = 1$ persists, $x = 1$ will continue to be stabilized. The situation is similar to the opening of a gap at the Fermi level in the Peierls instability of 1D chains, and is reminiscent to mode-locking in dynamical systems. A possible improvement of our argument, using homotopy concepts is under consideration.

3. Cusplike structure.

A semi-classical approach near an arbitrary rational flux p/q can be developed similarly [5, 10]. One can prove rigorously

Proposition 2. For a given rational value p/q of ν, the plot of the total energy $E(\phi, \nu)$ as a function of ϕ exhibits cusps at $\phi = (mq - p)/nq$ of flux values $(0 < \phi < 1)$, *i.e.* a dense set indexed by the integers m, n (gaps labels). Furthermore, at $\phi = \nu$, the slope difference $\{\partial E^+/\partial\phi - \partial E^-/\partial\phi\}$ is given by the width of the gap labelled by $m = 0$, $n = -1$. (Here we have adopted the notation $m - n\phi$ for the IDS inside the gap (m, n).) ◇

Proposition 3. Let $E_0(\nu) = E(\phi = \nu, \nu)$ be the ground-state energy; it is a smooth function of ν (namely differentiable at every order) except possibly at $\nu = 0$ and at every rational values $\nu = p/q$ for which the gap at the Fermi level closes. ◇

The proof of proposition 3, without being difficult, requires however an elaborate machinery of noncommutative geometry [12].

Regarding proposition 2, the following argument, valid at $\phi = p/q$, illustrates the heart of the proof (the extension to other cusps is immediate). Let us denote by $(\mu^+(\phi), \mu^-(\phi))$, the gap corresponding to an IDS equal to ϕ in the vicinity of $\phi = \nu$. At $\phi = \nu$, $\mu^+(\phi)$ (respectively, $\mu^-(\phi)$) is the top (respectively, the bottom) of the subband below (respectively, above) this gap. Thus for $\phi > \nu$, but $\phi \approx \nu$, the IDS is bigger than ν, whereas it is smaller for $\phi < \nu$. In order that the IDS be equal to ν (at $\phi > \nu$), the first LL at the top μ^+ of the last filled subband (the «valence band») must be partially filled. Similarly at $\phi < \nu$, the same argument implies that the first LL at the bottom $\mu^- > \mu^+$ of the next subband (the «conduction band») is partially filled. In particular, for $\phi > \nu$, we get

$$E(\phi, \nu) = E(\phi, \phi) - \{\mu^+ + O(\phi - p/q)\}(\nu - \phi)$$

for the first LL at μ^+ corresponds to the energy $\{\mu^+ + O(\phi - p/q)\}$, whereas $(\nu - \phi)$ corresponds to the fraction of it which is empty. Thus, the slopes $\partial E^{\pm}/\partial\phi$ at $\phi = \nu \pm 0$ are governed by the edge of the corresponding partially filled subband. This argument holds for every cusps corresponding to a jump of the Fermi energy, at absolute or local minima of E. In general we found the following simple result:

$$\left.\frac{\partial E^{\pm}}{\partial\phi}\right|_{\nu} = -\int_{-\infty}^{\mu^{\pm}(\phi)} \mathrm{d}\varepsilon \, \frac{\partial N(\varepsilon, \phi)}{\partial\phi}, \tag{10}$$

where $N(\varepsilon, \phi)$ refers for the IDS at energy ε and flux ϕ. A direct consequence of eq. (10) is

$$\left.\frac{\partial E^+}{\partial\phi}\right|_{\nu} - \left.\frac{\partial E^-}{\partial\phi}\right|_{\nu} = \frac{\partial N}{\partial\phi}(\mu^- - \mu^+). \tag{11}$$

Here $\partial N/\partial\phi$ is the integer labelling the gap just above μ^+. At this point two remarks are of order. Firstly, the general situation corresponds to asymmetric cusps: $\partial E^+/\partial\phi + + \partial E^-/\partial\phi \neq 0$ (see eq. (9)). Secondly, this result has been obtained for fixed N and fixed cell area. This has to be contrasted with the relevant discussion of ref. [13], relative to the analyticity of the energy under different conditions and for different problems.

To summarize, we have proved perturbatively the validity of the stabilization of the Fermi sea by the gaps, with an optimal flux corresponding to one flux quantum per fermion. The explicit cusplike structure (asymmetry, dense set of singularities, ...) of the energy as well as the smoothness of the ground-state energy have been made precise. Our method allows for the investigation of other problems (*i.e.* staggered flux, periodic flux, etc.). Results pertaining to this class of problems will be reported in the near future.

REFERENCES

[1] See for instance PRANGE R. E. and GIRVIN S. N. (Editors), *The Quantum Hall Effect* (Springer-Verlag, New York, N.Y.) 1987.

[2] CHEN Y. H., WILCZEK F., WITTEN E. and HALPERIN B., *Int. J. Mod. Phys. B*, **3** (1989) 1001; CANRIGHT G. S., GIRVIN S. N. and BRASS A., *Phys. Rev. Lett.*, **63** (1989) 2291, 2295.

[3] ANDERSON P. W., *Phys. Scr.*, T27 (1989) 660; WIEGMANN P. B., *Phys. Scr.*, T27 (1989) 160; LEDERER P., POILBLANC D. and RICE T. M., *Phys. Rev. Lett.*, **63** (1989) 1519.

[4] AZBELL M. YA., *Ž. Èksp. Teor. Fiz.*, **46** (1964) 929 (*Sov. Phys. JETP*, **19** (1964) 634); HOFSTADTER D. R., *Phys. Rev. B*, **14** (1976) 2239; CLARO F. H. and WANNIER G., *Phys. Rev. B*, **19** (1979) 6068; RAMMAL R., *J. Phys. (Paris)*, **46** (1985) 1345; CLARO F. H., *Phys. Status Solidi B*, **104** (1981) 31.

[5] For a comprehensive recent review, see BELLISSARD J., in *The Harald Bohr Centeray*, edited by C. BERG and F. FUGLEDE (The Royal Danish Acad. Sci., Copenhagen) 1989.

[6] ANDERSON P. W., in *Kathmandu Summer School Lectures* (1989), unpublished notes.

[7] HASEGAWA Y., LEDERER P., RICE T. M. and WIEGMANN P. B., *Phys. Rev. Lett.*, **63** (1989) 907; NOTI F. *et al.*, unpublished; LANTWIN C. J., unpublished; HASEGAWA Y. *et al.*, unpublished.

[8] MONTAMBAUX G., *Phys. Rev. Lett.*, **63** (1989) 1657.

[9] For previous attempts, see WILKINSON M., *J. Phys. A*, **17** (1984) 3459; WANG Y. Y., PANNETIER B. and RAMMAL R., *J. Phys. (Paris)*, **48** (1987) 2067 and references therein. Rigorous works can be found in: BELLISSARD J., in *Operators Algebra and its Applications*, edited by D. E. EVANS and M. TAKESAKI (Cambridge University Press, Cambridge) 1988 and also in ref. [5]; NENCIU G., unpublished; HELFFER B. and SJÖSTRAND J., to appear in *Mémories de la Soc. Math. de France* (1989).

[10] RAMMAL R. and BELLISSARD J., to appear in *J. Phys. (Paris)* (1990).

[11] PEIERLS R., *Surprise in Theoretical Physics* (Princeton University Press, Princeton, N.J.) 1979.

[12] BELLISSARD J. and RAMMAL R., to appear in *J. Phys. (Paris)* (1990).

[13] TESANOVIC Z., AXEL F. and HALPERIN B. I., *Phys. Rev. B*, **39** (1989) 8525.