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An algebraic semi-classical approach to Bloch electrons in a magnetic field

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Résumé. — En adoptant le point de vue de Heisenberg, on introduit une nouvelle méthode de quantification semi-classique, pour les électrons de Bloch sous champ magnétique. La structure du réseau est utilisée pour définir une structure algébrique. L'algèbre, dite de rotation, ainsi définie est non commutative, mais permet d'avoir un développement systématique à flux nul ainsi qu'à flux rationnel quelconque. L'ensemble des résultats connus sont retrouvés dans le cadre de notre formalisme, sans faire appel à la notion de fonction d'onde telle que dans la méthode WKB ou celle de l'équation du mouvement par exemple. Des nouveaux résultats, jusqu'au second ordre en flux sont donnés ainsi que des exemples simples pour illustrer la méthode algébrique.

Abstract. — Starting from Heisenberg's point of view, a semi-classical quantization method is introduced for 2D Bloch electrons in a magnetic field. The underlying lattice structure is used to define an algebraic structure. The (rotation) algebra so defined is non commutative, but allows for a systematic expansion of the magnetic energy levels, free energy, etc. near zero as well as an arbitrary rational flux. All previously derived results are recovered as special cases, but without involving wave function considerations (WKB, equation-of-motion methods, etc.). New results, up to second order in the magnetic flux, are explicitly derived and simple examples are used to illustrate our general algebraic formalism.

1. Introduction.

In recent years, many physical problems have been shown to be related to various aspects of the Landau level spectrum of Bloch electrons. Indeed, the motion of an electron in a crystal lattice in 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 and this for at least two reasons. First, because of its importance in various 2D physical interesting problems : Quantized Hall effect [1], quasi-1D conductor, anyon superconductivity [2], flux state model for high temperature superconductivity [3], superconducting networks [4], magnetoresistance of submicronic metallic networks [5], etc. The other reason stems from the recent advances in mathematics and mathematical physics : Schrödinger operators with almost periodic potentials [6], C* algebras of almost periodic operators [7], non commutative cohomology [8], etc.

In most cases, one can reduce the 2D problems into 1D quantum mechanics e.a. almost Mathieu equations [9] or Harper equation.

More recently, the computation of the spectrum boundaries motivated some progress for this class of problems. Using semi-classical ideas, some new results have been derived [10-12]. In particular, the shape of the spectrum edge at arbitrary rational flux has been studied and the so-called Wilkinson-Rammal formula (see below) was derived. This extension of the semi-classical ideas [13] to finite flux is not so immediate [14]. On the other hand, the used methods were mainly non-trivial adaptations of WKB theory. Here, the notion of wave function is an essential one, and the main difficulty comes from the connection formula between different sectors (see Ref. [10] for instance). Furthermore, it is usually very difficult to go beyond the first order expansion. This serious limitation of the potential use of WKB methods motivated a purely algebraic approach, which has been developed by one of us [15]. This new formulation for 2D Bloch electrons in a magnetic field provides actually a powerful and elegant method. Unfortunately, the algebraic method calls for an elaborate machinary of non commutative geometry, which is not widely known in the physics community.

The purpose of this paper is to outline first and then use the algebraic approach in order to derive new results. To our knowledge, this is the first extensive use of this methodology. In this respect, other applications of this formalism are expected in the future. Accordingly, this paper is organized as follows. In section 2, we summarize the basic features of the method, with reference to mathematical literature when rigorous derivations of some results will be found. Section 3 is devoted to the implementation of this method in the case of zero flux (weak field expansion). In section 4, we generalize to the case of a national flux, where a new computational trick is used in order to push the expansion up to second order. The results as well as the procedure we used are best illustrated in terms of examples. For this reason, we give explicit examples through the length of this paper. Our conclusion section is the object of some remarks relative to the extension of this work to treat other new problems. For the sake of clarity, we limited our exposition to the quantization of magnetic energy levels. The calculations of the magnetic susceptibility, which includes both the de Haas-van Alphen effect and the steady susceptibility, are left out. However, a direct use of the results derived below, to the problem of the Fermi sea stabilization by the gaps, will be found in the next paper [16].

2. Algebraic Formalism [15].

In this section we introduce the algebraic formalism and the notation used in the next sections. Readers, which are familiar with this formalism, will ignore this section which is a sort of summary of previous works.

2.1 INTRODUCTORY EXAMPLE. — Let us consider the case of a tight-binding model on a simple square lattice. In absence of magnetic field, the Hamiltonian may be described by means of nearest-neighbours interactions :

$$H\psi(m, n) = \psi(m+1, n) + \psi(m-1, n) + \psi(m, n+1) + \psi(m, n-1) \qquad (2.1)$$

where $\psi(m, n)$ is the wave function at node (m, n). Adding a uniform magnetic field will result in changing the phase of each term in equation (2.1) :

$$H\psi(m, n) = e^{i\gamma_1(m, n)}\psi(m+1, n) + e^{-i\gamma_1(m-1, n)}\psi(m-1, n) + \\ + e^{i\gamma_2(m, n)}\psi(m, n+1) + e^{-i\gamma_2(m, n-1)}\psi(m, n-1) \qquad (2.2)$$

where $\gamma_\mu(m, n)$ denotes the line integral of the vector potential between the site (m, n) of the lattice and the point $(m+1, n)$ for $\mu = 1$ or $(m, n+1)$ if $\mu = 2$. In particular,

because the magnetic field is uniform, one must have :

$$\gamma_1(m, n) + \gamma_2(m+1, n) - \gamma_1(m, n+1) - \gamma_2(m, n) = 2\pi \frac{\phi}{\phi_0} \equiv \gamma \tag{2.3}$$

where $\phi_0 = hc/e$ is the quantum of flux and ϕ the flux through the unit cell. With Landau gauge (particular solution of Eq. (2.3)) :

$$\gamma_1(m, n) = 0, \quad \gamma_2(m, n) = \gamma m \tag{2.4}$$

the Hamiltonian H commutes with space translations along the n-direction and the solutions of Schrödinger equation $H\psi = E\psi$ will have the form :

$$\psi(m, n) = e^{ikn}\, \phi(n) . \tag{2.5}$$

This leads to the well known Harper's equation :

$$\phi(n+1) + \phi(n-1) + 2\cos(\gamma . n + k) . \phi(n) = E\phi(n) . \tag{2.6}$$

A fundamental remark in the algebraic formalism is that equation (2.2) can be written in an algebraic way, by introducing the following two unitaries U and V :

$$\begin{aligned} U\psi(m, n) &= e^{-i\gamma_1(m-1, n)}\, \psi(m-1, n) \\ V\psi(m, n) &= e^{-i\gamma_2(m, n-1)}\, \psi(m, n-1) . \end{aligned} \tag{2.7}$$

They satisfy the following commutation relation :

$$UV = e^{i\gamma} VU, \quad \gamma = 2\pi\alpha \equiv 2\pi \frac{\phi}{\phi_0} . \tag{2.8}$$

The Almost-Mathieu Hamiltonian H can then be written simply as :

$$H = U + U^* + V + V^* . \tag{2.9}$$

This example illustrates a general property. In general, it is possible to show that the Hamiltonian for 2D Bloch electrons (see below) in a uniform magnetic field belongs to the C*-Algebra generated by U and V.

2.2 ROTATION ALGEBRA $\mathcal{A}(\alpha)$: BRIEF ACCOUNT. — The operators U and V of the previous example generate a C*-Algebra $\mathcal{A}(\alpha)$ called the rotation algebra ([1]). Introduced for purely mathematical reasons, $\mathcal{A}(\alpha)$ constitutes a remarkable object because it is non-commutative whenever α is irrational. In recent years, $\mathcal{A}(\alpha)$ and its generalization have been used to get general properties of the energy spectrum : gap labelling, integrated density of states, current correlations, etc. More recently, the definition of a differential structure (see below) permitted to provide a mathematical framework to prove the quantum Hall effect and for a detailed study of Harper's equation.

In what follows, we will give a brief exposition of the rotation algebra $\mathcal{A}(\alpha)$, detailed definitions are the object of the next subsection.

Consider the situation of a 2D Bloch electron in a magnetic field :

$$H = \frac{1}{2m} \sum_{i=1,2} [\mathbf{P}_i - e\mathbf{A}_i(\mathbf{Q})]^2 + V(\mathbf{Q}) \tag{2.10}$$

([1]) The reason for using the terminology « rotation algebra » can be seen as follows. There is one representation where the action of V is a simple multiplication by $\exp(2i\pi\alpha)$ and this is nothing else than the rotation with angle α. For more details, see M. R. Rieffel, « irrational rotation $\mathbb{C}^*$-Algebra » ; Short Communication to the congress of Mathematicians (1978).

where $\mathbf{Q} = (Q_1, Q_2)$ is the position operator, $\mathbf{P} = (P_1, P_2)$ is the momentum operator, $\mathbf{A} = (A_1, A_2)$ the magnetic vector potential and V is a periodic potential. The kinetic part of H is no longer translation invariant because the vector potential breaks the translation symmetry. However, adding a phase factor to the translation operator, we get the following « magnetic translations » :

$$[U(\mathbf{a})\,\psi](\mathbf{Q}) = \exp(i\pi eB\mathbf{Q} \times \mathbf{a})\,.\,\psi(\mathbf{Q} - \mathbf{a}) \tag{2.11}$$

where $\mathbf{Q} \times \mathbf{a} \equiv Q_1 a_2 - Q_2 a_1$ if $\mathbf{Q} = (Q_1, Q_2)$ and $\mathbf{a} = (a_1, a_2)$. Now, if $\mathbf{a}$ is a period of V, H commutes with $U(\mathbf{a})$. The algebra generated by the magnetic translations $U(\mathbf{a})$, is the natural extension of the example described in the introduction, which is nothing else than a lattice version of this algebra.

Very important notions such as the trace (per unit volume) and the differential structure have been introduced. Roughly, the trace τ per unit volume and the differential structure are entirely defined by the following conditions :

$$\tau(U^m V^n) = \delta_{n,0}\,\delta_{m,0}\,, \quad \tau(\mathbb{1}) = 1 \tag{2.12}$$

$$\partial_1 U = 2i\pi U\,, \quad \partial_2 V = 2i\pi V\,; \quad \partial_2 U = \partial_1 V = 0\,. \tag{2.13}$$

It turns out that these notions are very useful in practice. Let us mention the integrated density of states (IDS) : $\mathcal{N}(E)$ equal the number (per unit volume) of eigenvalues below E :

$$\mathcal{N}(E) = \tau(P(E)) \tag{2.14}$$

where P represents the eigenprojection of the Hamiltonian H on energies smaller than E.

Another example is provided by the Chern character $\mathrm{Ch}(P)$ of a given projection P in the algebra :

$$\mathrm{Ch}(P) = \frac{1}{2i\pi}\,\tau\{P[\partial_1 P, \partial_2 P]\}\,. \tag{2.15}$$

In particular, the Hall conductivity at zero temperature is given by

$$\sigma_H = \frac{e^2}{h}\,\mathrm{Ch}(P_F)\,. \tag{2.16}$$

Here, P_F is the eigenprojector on energies smaller than or equal to the Fermi energy E_F. The conditions of validity of equation (2.16) are discussed in reference [7].

A direct application of equations (2.14) and (2.15) is the proof of the Streda [1] formula :

$$\sigma_H = e\,\partial\mathcal{N}(E)/\partial B \tag{2.17}$$

where B is the magnetic field. Equation (2.17) relates the Hall conductivity σ_H to the integrated density of states within the gaps.

2.3 PRECISE DEFINITIONS AND COMPUTATIONAL TOOLS. — a) *Why the rotation algebra ?* — The basic remark behind the introduction of the algebra $\mathcal{A}(\alpha)$ is already clear in the absence of the potential V. Indeed the conventional way in describing the one electron Hamiltonian for a Bloch electron in a magnetic field is to make the substitution $\mathbf{P} \to \mathbf{K} = \mathbf{P} - e\mathbf{A}$, where $\mathbf{P}$ is the momentum operator and $\mathbf{A}$ satisfies :

$$\partial_1 \mathbf{A}_2 - \partial_2 \mathbf{A}_1 = \mathbf{B}\,. \tag{2.18}$$

For $V = 0$ in equation (2.10), the spectrum of H is immediately calculated. It comes from the remark that $\mathbf{K}$ obey to the canonical commutation relations, namely :

$$[K_1, K_2] = iehB/2\pi . \tag{2.19}$$

Therefore H becomes the energy operator for a harmonic oscillator. The spectrum is then given by : $E_n = (2n + 1) E_0$, $n = 0, 1, 2, \ldots$ This feature of the problem remains true when $V \neq 0$ and this for strong as well as weak field respectively.

In strong field limit, it is useful to introduce a new set of canonical variables, besides $\mathbf{K}$. We first choose a symmetric gauge :

$$A_\mu(\mathbf{Q}) = -\frac{B}{2} \varepsilon_{\mu\nu} Q_\nu ; \quad \varepsilon_{12} = -\varepsilon_{21} = 1 , \quad \varepsilon_{11} = \varepsilon_{22} = 0 . \tag{2.20}$$

If we set $k_\mu = \frac{1}{2} Q_\mu + \frac{1}{eB} \varepsilon_{\mu\nu} P_\nu$, we get :

$$[K_\mu, k_\nu] = 0 , \quad [k_1, k_2] = -ih/2\pi eB \tag{2.21}$$

and

$$Q_\mu = k_\mu - \frac{1}{eB} \varepsilon_{\mu\nu} K_\nu . \tag{2.22}$$

The expansion of V in Fourier series, shows that [17] the band effective Hamiltonian belongs to the $\mathbb{C}^*$ Algebra generated by the unitary operators :

$$U = \exp(i \langle \mathbf{b}_1 | \mathbf{k} \rangle) , \quad V = \exp(i \langle \mathbf{b}_2 | \mathbf{k} \rangle) \tag{2.23}$$

where $\mathbf{b}_1$, $\mathbf{b}_2$ are the generators of the reciprocal lattice Γ^*. They satisfy : $UV = e^{2i\pi/\alpha} VU$, where $\alpha = \phi/\phi_0$. Here ϕ is the flux through the unit cell of the Bravais lattice Γ. In general U and V appear in the combination

$$W(m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2) \equiv e^{-i\pi \frac{1}{\alpha} m_1 m_2} U^{m_1} V^{m_2} . \tag{2.24}$$

In the weak field limit, we have a dual situation, where the effective Hamiltonian belongs to the $\mathbb{C}^*$ Algebra generated by $\exp(i \langle \mathbf{a} | \mathbf{K} \rangle)$'s, namely by two unitaries U and V defined by

$$U = \exp(i \langle \mathbf{a}_1 | \mathbf{K} \rangle) , \quad V = \exp(i \langle \mathbf{a}_2 | \mathbf{K} \rangle) , \quad UV = e^{2i\pi\alpha} VU . \tag{2.25}$$

Here $\mathbf{a}_1$ and $\mathbf{a}_2$ are the generators of the Bravais lattice Γ. Furthermore, U and V appear always in the combinations :

$$W(m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2) = e^{-i\pi\alpha m_1 m_2} U^{m_1} V^{m_2} . \tag{2.26}$$

So, every operator of interest for us can actually be expanded in terms of trigonometric polynomials in two unitaries U and V such that $UV = e^{2i\pi\alpha} VU$.

b) *Topology of* $\mathcal{A}(\alpha)$. — Of main interest for us, are the following properties of $\mathcal{A}(\alpha)$:

i) $\mathcal{A}(\alpha) = \mathcal{A}(\alpha + 1)$: gauge invariance.

ii) If W_1 and W_2 are two $q \times q$ unitary matrix such that $W_1 W_2 = e^{2i\pi p/q} W_2 W_1$, $W_1^q = W_2^q = 1$, then $\mathcal{A}(p/q)$ is isomorphic to the set of matrix valued functions $F(\mathbf{k})$ over $\mathbb{R}^2$ such that :

$$(W_1^{m_2} W_2^{-m_1}) F(\mathbf{k}) (W_1^{m_2} W_2^{-m_1})^* = F(\mathbf{k} + \mathbf{m}) , \quad \mathbf{m} \in \mathbb{Z}^2 . \tag{2.27}$$

iii) A trace τ per unit volum on $\mathcal{A}(\alpha)$ is entirely defined by :

$$\tau(U^{m_1} V^{m_2}) = 0 \quad \text{if} \quad \mathbf{m} \neq 0\,, \quad \tau\,(\mathbb{1}) = 1\,. \tag{2.28}$$

Furthermore, if P is a projection of $\mathcal{A}(\alpha)$, there is a unique integer n such that $\tau(P) = \{n\alpha\}$ where $\{x\}$ denotes the fractional part of x [18].

c) *Differential structure.* — The rotation algebra $\mathcal{A}(\alpha)$ can actually be viewed as a non-commutative 2D torus by identifying U and V with the coordinate functions. This allows to define two derivatives as follows :

$$\partial_1 U = 2\,i\pi U\,, \quad \partial_2 V = 2\,i\pi V\,; \quad \partial_2 U = \partial_1 V = 0\,.$$

These derivatives commute. Furthermore, we see that U and V become analogous to the coordinate functions $e^{2\,i\pi x_\mu}$ ($\mu = 1, 2$) of a 2D-torus, if the trace τ is replaced by normalized Haar measure and if the ∂_μ's represent the usual partial derivatives.

Let now P be a projection of $\mathcal{A}(\alpha)$. The Chern class of P is defined by analogy with the 2-torus as :

$$\mathrm{Ch}(P) = \frac{1}{2\,i\pi}\,\tau(P[\partial_1 P, \partial_2 P])\,. \tag{2.29}$$

The main result concerning the Chern class is the following : if P is a projection of $\mathcal{A}(\alpha)$, its Chern class is an integer.

d) *Ito-like derivative.* — By considering the set $\mathcal{A} = \{\mathcal{A}(\alpha), \alpha \in \mathbb{R}\}$, one can define the derivation with respect to α. More precisely, let A be a polynomial :

$$A = \sum_{m} a(\mathbf{m}\,;\,\alpha)\,W(\mathbf{m})\,, \quad \text{with} \quad W(m_1, m_2) = e^{i\pi\alpha m_1 m_2}\,U^{m_1} V^{-m_2}\,.$$

The operator ∂ is defined by

$$\partial A = \sum_{m} \frac{\partial a(\mathbf{m}\,;\,\alpha)}{\partial\alpha}\,W(\mathbf{m})\,.$$

This operation satisfies the following rules :

i) $$\partial(AB) = \partial A\,.\,B + A\,.\,\partial B + \frac{i}{4\,\pi}\,\{\partial_1 A\,\partial_2 B - \partial_2 A\,\partial_1 B\} \tag{2.30}$$

ii) if A^{-1} exists, then :

$$\partial(A^{-1}) = -\,A^{-1}\left\{\partial A + \frac{i}{4\,\pi}\,(\partial_1 A\,.\,A^{-1}\,.\,\partial_2 A - \partial_2 A\,.\,A^{-1}\,.\,\partial_1 A)\right\} A^{-1}\,. \tag{2.31}$$

In particular, one can show (Streda's formula) :

$$\frac{\partial}{\partial\alpha}\,\tau(P) = \mathrm{Ch}\;(P) \tag{2.32}$$

for a projection P.

2.4 SIMPLE EXAMPLES. — The following examples illustrate the notions introduced in the preceding section.

a) *Rectangular lattice.* — Introducting an anisotropy between the horizontal and vertical axis, does not change the form of the Hamiltonian :

$$H = (U + U^*) + \mu (V + V^*), \quad UV = e^{2i\pi\alpha} VU . \tag{2.33}$$

Here μ measures the anisotropy ratio of the coupling constants in the vertical *versus* the horizontal directions. The corresponding 1D equation (analogous of Eq. (2.6)) also represents the effective Hamiltonian for a tight-binding representation of the effect of a charge density wave in a 1D conductor provided μ represents the strength of the Peierls instability.

The energy operator H is the quantized version of $\mathcal{H}(\mathbf{k}, \alpha)$ obtained by replacing U by e^{ik_1}, V by e^{ik_2}, $W(m_1, m_2)$ correspond in general to $e^{(im_1 k_2 - m_2 k_1)}$. The classical Hamiltonian is then given by

$$\mathcal{H}(\mathbf{k}, \alpha) = 2 \cos k_1 + 2 \mu \cos k_2 . \tag{2.34}$$

b) *Generalized square lattice.* — In this case (Fig. 1b), H can be written as

$$H = U + V + \mu (X + Y) + \text{h.c.} \tag{2.35}$$

where μ is the ratio of the hopping matrix elements between $n.n.n$ and $n.n$ sites : $\mu = t_2/t_1$. Using the notations of (Fig. 1b) one gets :

$$UV = e^{2i\pi\alpha} VU, \quad UVY^{-1} = e^{2i\pi\alpha}$$

and this leads to :

$$Y = UV e^{-i\pi\alpha} = VU e^{i\pi\alpha}, \quad X = UV^* e^{i\pi\alpha} = V^* U e^{-i\pi\alpha} \tag{2.36}$$

and

$$H = U + V + \mu (e^{-i\pi\alpha} V^* + e^{i\pi\alpha} V) U + \text{h.c.} \tag{2.37}$$

The classical version of H exhibits an explicit dependence on α :

$$\mathcal{H}(\mathbf{k}, \alpha) = 2 \cos k_1 + 2 \cos k_2 + 2 \mu \cos k_1 . 2 \cos (k_2 + \pi\alpha) . \tag{2.38}$$

c) *Triangular lattice.* — In this case, one obtains :

$$H = (U + V + Y) + \text{h.c.} ,$$

and, using $Y = VU e^{i\pi\alpha}$, one deduces :

$$H = (U + V + VU e^{i\pi\alpha}) + \text{h.c.} \tag{2.39}$$

The classical counterpart of H is given by

$$\mathcal{H}(\mathbf{k}, \alpha) = 2 \cos k_1 + 2 \cos k_2 + 2 \cos (k_1 + k_2 + \pi\alpha) . \tag{2.40}$$

d) *Two flux triangular lattice.* — Assuming a flux η for up triangles and $\phi - \eta$ for down triangles, one obtains :

$$H = (T_1 + T_2 + T_3) + \text{h.c.}, \quad \text{with} \quad T_1 T_2 = e^{i\phi} T_2 T_1 \quad \text{and} \quad T_1 T_2 T_3 = e^{i\eta} .$$

Using the above notations : $W(m_1, m_2) = T_2^{m_1} T_1^{-m_2} e^{-i\frac{\gamma}{2} m_1 m_2}$, one deduces ($\gamma = 2\pi\alpha$).

$$T_3 = T_2^{-1} T_1 e^{i\eta} = W(-1, 1) e^{i(\eta - \gamma/2)} .$$

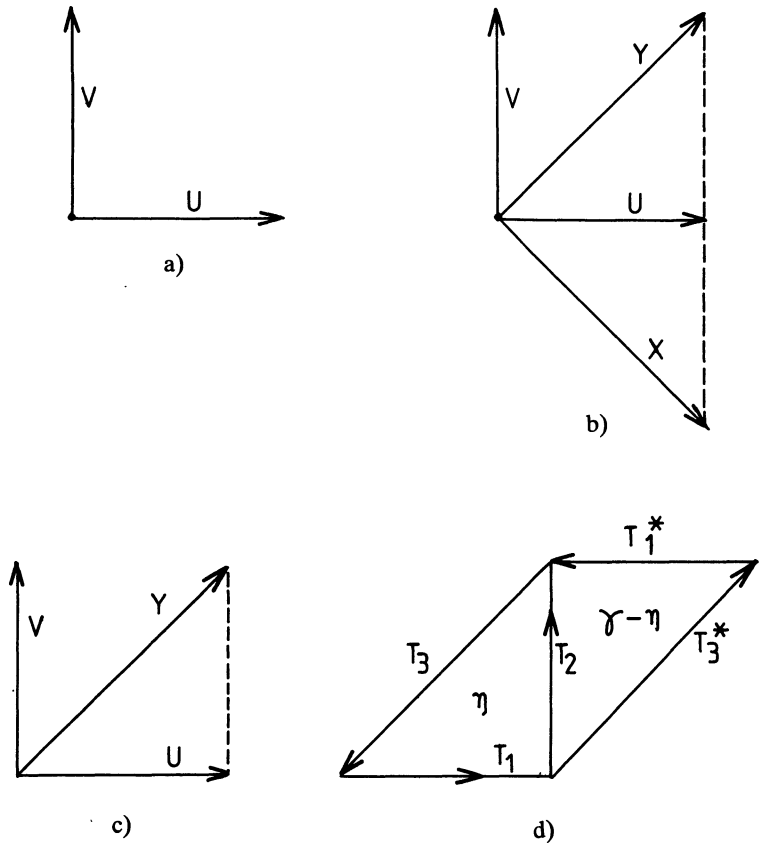

Fig. 1. — Notations used in the text for the magnetic translation operators. (a) simple square lattice, (b) generalized square lattice, (c) triangular lattice, (d) two flux triangular lattice.

The classical version of H is then

$$\mathcal{H}(\mathbf{k}) = 2\cos k_1 + 2\cos k_2 + 2\cos\left(k_1 + k_2 + \frac{\gamma}{2} - \eta\right). \tag{2.41}$$

Let us mention that the spectrum of this model has been investigated by one of us, where new qualitative features have been obtained [19].

3. Semi-Classical Expansion at Weak Magnetic Field.

In this section, we outline first the quantization procedure at weak magnetic field. Previously obtained results are then recalled and new results are derived.

3.1 QUANTIZATION AND FIRST ORDER EXPANSION. — In reference [7], the following result has been obtained. Let $\mathcal{H}(\mathbf{k}\,;\,\alpha)$ be a continuous function of the real variables $\mathbf{k} = (k_1, k_2)$ and α. Assume that $\mathcal{H}(\mathbf{k}, \alpha)$ is periodic with respect to $\mathbf{k}$, of period 2π in each component of $\mathbf{k}$. Let $\mathcal{H} = \sum_m h(\mathbf{m}\,;\,\alpha)\, e^{i\mathbf{k}\times\mathbf{m}}$ be the Fourier expansion of $\mathcal{H}$ (with $\mathbf{k}\times\mathbf{m} = k_1 m_2 - k_2 m_1$) and assume that for each α of interest, $\mathcal{H}(\mathbf{k}\,;\,\alpha)$ has a unique regular minimum in each

cell of period. Without loss of generality one can assume that this minimum is located at $\mathbf{k} = 0$ for $\alpha = 0$ and $\mathcal{H}(\mathbf{0}\,;0) = 0$. Correspondingly, we define the quantized of $\mathcal{H}$ as the following element of the algebra $\mathcal{A}(\alpha)$:

$$H(\alpha) = \sum_{m} h(\mathbf{m}\,;\alpha)\, W(\mathbf{m}),\ W(\mathbf{m}) = \mathrm{e}^{i\pi\alpha m_1 m_2}\, U^{m_1} V^{m_2}. \tag{3.1}$$

The ground state energy $E(\alpha)$ is defined as the infinum of the spectrum of $H(\alpha)$ in $\mathcal{A}(\alpha)$. In the limit $\alpha \sim 0$, the asymptotic behavior of $E(\alpha)$ (semi-classical expansion) is given by the following :

$$E(\alpha) = 2\pi\,|\alpha|\cdot\left[\det\left(\frac{1}{2}\frac{\partial^2 H}{\partial k_i\,\partial k_j}(\mathbf{0}\,;0)\right)\right]^{1/2} + \alpha\,\frac{\partial\mathcal{H}}{\partial\alpha}(\mathbf{0}\,;0) + \cdots \tag{3.2}$$

More generally, the « Landau » levels are given by ($n = 0, 1, 2, \ldots$) :

$$E_n(\alpha) = (2n+1)\cdot 2\pi\,|\alpha|\cdot\left[\det\frac{1}{2}D^2 H(\mathbf{0}\,;0)\right]^{1/2} + \alpha\cdot\frac{\partial\mathcal{H}}{\partial\alpha}(\mathbf{0}\,;0) + \cdots \tag{3.3}$$

The accuracy of this « harmonic oscillator » result is discussed in reference [7]. One notices the occurrence of the last new term which is due to the explicit dependence of $\mathcal{H}$ on α. In some sense, equation (3.3) is the most general result, to first order in α.

3.2 AN ILLUSTRATIVE EXAMPLE. — In order to introduce the general formalism, let us consider the case of Harper's equation :

$$H = U + U^* + V + V^* \tag{3.4}$$

with $UV = \mathrm{e}^{2i\pi\alpha}\, VU$. H is the quantized of $\mathcal{H}(\mathbf{k})$ obtained as described before ($U \to \mathrm{e}^{ik_1}$, $V \to \mathrm{e}^{ik_2}$) :

$$\mathcal{H}(\mathbf{k}) = 2\cos k_1 + 2\cos k_2\,. \tag{3.5}$$

The minimum of $\mathcal{H}(\mathbf{k})$ is reached at $k_1 = k_2 = \pi$. Near this critical point $\mathbf{k}_c = (\pi, \pi)$ the quantized of $\mathcal{H}$ results from the substitution : $\mathbf{k} \to \mathbf{k}_c + \gamma^{1/2}\mathbf{K}$, where $\mathbf{k} = (k_1, k_2)$ and K_μ are the components of the momentum operator ($\mu = 1, 2$). K_1 and K_2 are normalized such as :

$$[K_1, K_2] = i\,. \tag{3.6}$$

Therefore, H becomes :

$$H = -2\cos(\gamma^{1/2}K_1) - 2\cos(\gamma^{1/2}K_2)\,. \tag{3.7}$$

For vanishing γ, one can expand (Eq. (3.7)) in powers of γ. To order γ^2, one obtains : $H = -4 + \gamma h$, with

$$h = (K_1^2 + K_2^2) - \frac{\gamma}{12}(K_1^4 + K_2^4)\,. \tag{3.8}$$

Therefore, to first order in γ, one recovers the Landau levels structure

$$E_n = -4 + \gamma(2n+1) + 0(\gamma^2),\quad n = 0, 1, 2, \ldots \tag{3.9}$$

which is best described in terms of harmonic oscillator operators :

$$a = (K_1 + iK_2)/\sqrt{2}\,, \quad a^* = (K_1 - iK_2)/\sqrt{2}\,, \quad \text{with} \quad [a, a^*] = 1$$

and the eigenstates $|n\rangle = \dfrac{a^{*n}}{(n!)^{1/2}}\,|0\rangle$. In this respect, it is useful to recall the following rules : $a|n\rangle = n^{1/2}|n-1\rangle$, $a^*|n\rangle = (n+1)^{1/2}\,|n+1\rangle$ and $a^*a|n\rangle = n|n\rangle$. Considering the second part of equation (3.9) as a perturbation to the harmonic oscillator, one deduces the eigenvalues e_n of h as

$$e_n = (2n+1) - \frac{\gamma}{12}\,\langle n|K_1^4 + K_2^4|n\rangle + 0(\gamma^2)\,. \tag{3.10}$$

The matrix elements in equation (3.10) are simply obtained (see Appendix A) as :

$$\langle n|K_1^4|n\rangle = \langle n|K_2^4|n\rangle = \frac{3}{8}\,(1 + (1+2n)^2)$$

and this leads to :

$$E_n = -4 + (2n+1)\,\gamma - \frac{\gamma^2}{16}\,(1 + (1+2n)^2) + 0(\gamma^3)\,. \tag{3.11}$$

Next order terms in equation (3.11) can be calculated (see § 3.3) in a systematic way. Notice for the moment the absence of terms $0(\gamma^{1/2})$, $0(\gamma^{3/2})$, etc.

3.3 GENERAL CASE. — The result obtained above, can be generalized such as to include (Eq. (3.11)) as a limiting case. In fact, assuming the following normal form of the classical version $\mathcal{H}(\mathbf{k})$ of H :

$$\mathcal{H}(\mathbf{k}) = \mathcal{H}(\mathbf{0}) + \frac{\omega}{2}\,(k_1^2 + k_2^2) + 0(|\mathbf{k}|^3)\,, \quad \mathbf{k} \to \mathbf{0}\,, \quad \omega \neq 0 \tag{3.12}$$

then the following formula for E_n holds :

$$E_n = \mathcal{H}(\mathbf{0}) + \gamma\,\frac{\omega}{2}\,(2n+1) + \frac{\gamma^2}{64}\,\Delta^2\mathcal{H}(\mathbf{0})\cdot[1 + (1+2n)^2] -$$

$$- \frac{\gamma^2}{288\,\omega}\,[9(3n^2+3n+1)\,.\,|\Delta\,\partial\mathcal{H}(\mathbf{0})|^2 + (3n^2+3n+2)\,.\,|\partial^3\mathcal{H}(\mathbf{0})|^2] + 0(\gamma^3) \tag{3.13}$$

with

$$\partial \equiv \partial/\partial k_1 - i\partial/\partial k_2\,, \quad \bar{\partial} = \partial/\partial k_1 + i\partial/\partial k_2 \quad \text{and} \quad \partial\bar{\partial} = \Delta = \partial^2/\partial k_1^2 + \partial^2/\partial k_2^2\,.$$

This formula holds for an arbitrary 2D lattice, even in the case where $\mathcal{H}(\mathbf{k})$ exhibits an explicit dependence on the flux (see examples below).

The proof of equation (3.13) starts from the following expression of $\mathcal{H}(\mathbf{k})$:

$$\mathcal{H}(\mathbf{k}) = \sum_m h(m)\exp(i(m_1 k_2 - m_2 k_1))\,, \quad \mathbf{k} = (k_1, k_2) \tag{3.14}$$

we assume that $\mathcal{H}(\mathbf{0})$ is real and corresponds to a minima of $\mathcal{H}(k)$, where the second order derivative matrix $(\partial_\mu\,\partial_\nu\,\mathcal{H}(\mathbf{0}))_{\mu\nu}$ is positive definite. More precisely, without loss of generality, we assume up to a canonical change of coordinates : $\partial_\mu\,\partial_\nu\mathcal{H}(\mathbf{0}) = \omega\,\delta_{\mu\nu}$,

$\omega > 0$. The quantized version of $\mathcal{H}(\mathbf{k})$ is obtained by putting: $k_\mu \to \sqrt{\gamma}\, K_\mu$, where K_1 and K_2 are two self-adjoint operators with $[K_1, K_2] = i$. The expansion of H reads:

$$H = \sum_m h(m) \exp[i(m_1 K_2 - m_2 K_1)\, \gamma^{1/2}]$$

$$= \mathcal{H}(\mathbf{0}) + \gamma^{1/2} \partial_\mu \mathcal{H}(\mathbf{0}) \cdot K_\mu + \frac{\gamma}{2} \partial_\mu\, \partial_\nu \mathcal{H}(\mathbf{0}) \cdot K_\mu\, K_\nu + \cdots \tag{3.15}$$

The critical point is located at $\mathbf{k}_c = 0$, and $\partial_\mu \mathcal{H}(\mathbf{0}) = 0$. To order γ^2 one then obtains:

$$H = \mathcal{H}(\mathbf{0}) + \frac{\gamma}{2!} \partial_\mu\, \partial_\nu \mathcal{H}(\mathbf{0}) \cdot K_\mu\, K_\nu + \frac{\gamma^{3/2}}{3!} [\partial_{\mu 1}\, \partial_{\mu 2}\, \partial_{\mu 3} \mathcal{H}(\mathbf{0})] \cdot K_{\mu 1}\, K_{\mu 2}\, K_{\mu 3}$$

$$+ \frac{\gamma^2}{4!} [\partial_{\mu 1}\, \partial_{\mu 2}\, \partial_{\mu 3}\, \partial_{\mu 4} \mathcal{H}(\mathbf{0})] \cdot K_{\mu 1}\, K_{\mu 2}\, K_{\mu 3}\, K_{\mu 4} + \cdots$$

$$\equiv \mathcal{H}(\mathbf{0}) + \frac{\gamma}{2} (\partial_\mu\, \partial_\nu \mathcal{H}(\mathbf{0}) \cdot K_\mu\, K_\nu + V) \tag{3.16}$$

where $V = 0(\gamma^{1/2})$.

At the lowest order in γ, the dominant part is $H_0 = \partial_\mu\, \partial_\nu \mathcal{H}(\mathbf{0}) \cdot K_\mu\, K_\nu$ which is trivially diagonalized. Indeed, making an appropriate change of variable on $\mathbf{k}$, one can always be reduced to the case $H_0 = \omega (K_1^2 + K_2^2)$, with $\omega = |\det (\partial_\mu\, \partial_\nu \mathcal{H}(\mathbf{0}))|^{1/2} \times \text{sign}\, (\partial^2 \mathcal{H})$. Here sign $\partial^2 \mathcal{H} > 0$. At this order, one gets:

$$E_n^{(0)} = (2n + 1)\, \omega\,. \tag{3.17}$$

To first order in the perturbation, one has:

$$E_n^{(1)} = \langle n | V | n \rangle \tag{3.18}$$

and the next order is given by:

$$E_n^{(2)} = \sum_{n' (\neq n)} \frac{|\langle n | V | n' \rangle|^2}{2\, \omega\, (n - n')}\,. \tag{3.19}$$

From equation (3.16), V assumes the following form:

$$V = \frac{\gamma^{1/2}}{3} \partial_{\mu 1}\, \partial_{\mu 2}\, \partial_{\mu 3} \mathcal{H}(\mathbf{0}) \cdot K_{\mu 1}\, K_{\mu 2}\, K_{\mu 3} + \frac{\gamma}{12} \partial_{\mu 1}\, \partial_{\mu 2}\, \partial_{\mu 3}\, \partial_{\mu 4} \mathcal{H}(\mathbf{0}) \cdot K_{\mu 1}\, K_{\mu 2}\, K_{\mu 3}\, K_{\mu 4}$$

$$\equiv \frac{\gamma^{1/2}}{3} V_{1/2} + \frac{\gamma}{12} V_1\,. \tag{3.20}$$

Therefore, in the calculation of $E_n^{(2)}$ one can neglect $\frac{\gamma}{12} V_1$ and consider only $\frac{\gamma^{1/2}}{3} V_{1/2}$.

a) *Calculation of* $E_n^{(1)}$. — For symmetry reasons, $\langle n | K_{\mu 1}\, K_{\mu 2}\, K_{\mu 3} | n \rangle = 0$ and then only $\frac{\gamma}{12} V_1$ contributes to $E_n^{(1)}$:

$$E_n^{(1)} = \frac{\gamma}{12} \langle n | K_{\mu 1}\, K_{\mu 2}\, K_{\mu 3}\, K_{\mu 4} | n \rangle \cdot \partial_{\mu 1}\, \partial_{\mu 2}\, \partial_{\mu 3}\, \partial_{\mu 4} \mathcal{H}(0)\,. \tag{3.21}$$

Giving the symmetry of the tensor $\partial_{\mu 1}\, \partial_{\mu 2}\, \partial_{\mu 3}\, \partial_{\mu 4} \mathcal{H}(\mathbf{0})$ in μ_1, μ_2, μ_3 and μ_4, it is convenient to use

$$R_{\mu 1\, \mu 2\, \mu 3\, \mu 4} \equiv \sum_{\sigma \in S_4} K_{\mu_{\sigma(1)}} K_{\mu_{\sigma(2)}} K_{\mu_{\sigma(3)}} K_{\mu_{\sigma(4)}}$$

where σ belongs to the symmetric group S_4. Therefore,

$$\frac{12}{\gamma} E_n^{(1)} = \langle n | K_1^4 | n \rangle \cdot \partial_1^4 \mathcal{H}(\mathbf{0}) + \langle n | K_2^4 | n \rangle \cdot \partial_2^4 \mathcal{H}(\mathbf{0}) + \langle n | R_{3,1} | n \rangle \cdot \partial_1^3 \partial_2 \mathcal{H}(\mathbf{0}) + \langle n | R_{2,2} | n \rangle \cdot \partial_1^2 \partial_2^2 \mathcal{H}(\mathbf{0}) + \langle n | R_{1,3} | n \rangle \cdot \partial_1 \partial_2^3 \mathcal{H}(\mathbf{0}) \tag{3.22}$$

where, we have introduced the symmetric polynomials :

$$R_{3,1} = K_1^3 K_2 + K_1^2 K_2 K_1 + K_1 K_2 K_1^2 + K_2 K_1^3,$$
$$R_{2,2} = K_1^2 K_2^2 + K_1 K_2 K_1 K_2 + K_2 K_1^2 K_2 + K_1 K_2^2 K_1 + K_2 K_1 K_2 K_1 + K_2^2 K_1^2,$$
$$R_{1,3} = K_1 K_2^3 + K_2 K_1 K_2^2 + K_2^2 K_1 K_2 + K_2^3 K_1 .$$

Using the commutation relation $[K_1, K_2] = i$, one can calculate :

$$\langle n | K_1 K_2 + K_2 K_1 | n \rangle = 0$$
$$\langle n | K_1^2 K_2^2 + K_2^2 K_1^2 | n \rangle = \frac{1}{4} [(2n+1)^2 - 3]$$
$$\langle n | K_1^3 K_2 | n \rangle = i \frac{3}{4} (2n+1) .$$

This yields to :

$$\langle n | R_{1,3} | n \rangle = \langle n | R_{3,1} | n \rangle = 0$$
$$\langle n | R_{2,2} | n \rangle = \frac{3}{4} [1 + (1+2n)^2] ,$$

and then

$$E_n^{(1)} = \frac{\gamma}{32} [1 + (1+2n)^2] \cdot (\partial_1^2 + \partial_2^2)^2 \mathcal{H}(\mathbf{0}) . \tag{3.23}$$

b) *Calculation of* $E_n^{(2)}$. — The computation of $E_n^{(2)}$ requires the calculation of the matrix elements of $V_{1/2}$ given by : $V_{1/2} = \partial_{\mu 1} \partial_{\mu 2} \partial_{\mu 3} \mathcal{H}(\mathbf{0}) \cdot K_{\mu 1} K_{\mu 2} K_{\mu 3}$. The only non vanishing elements are $\langle n | V_{1/2} | n \pm 1 \rangle$ and $\langle n | V_{1/2} | n \pm 3 \rangle$. Proceeding as before, one obtains :

$$\langle n | V_{1/2} | n-1 \rangle = \langle n-1 | V_{1/2} | n \rangle^* = \frac{3 n^{3/2}}{2\sqrt{2}} \Delta \, \bar{\partial} \mathcal{H}(\mathbf{0}) ,$$
$$\langle n | V_{1/2} | n-3 \rangle = \langle n-3 | V_{1/2} | n \rangle^* = \left[\frac{n(n-1)(n-2)}{8} \right]^{1/2} \Delta \, \bar{\partial}^3 \mathcal{H}(\mathbf{0}) ,$$
$$\langle n | V_{1/2} | n+3 \rangle = \left[\frac{(n+1)(n+2)(n+3)}{8} \right]^{1/2} \Delta \, \partial^3 \mathcal{H}(\mathbf{0}) ,$$
$$\langle n | V_{1/2} | n+1 \rangle = \frac{3(n+1)^{3/2}}{2\sqrt{2}} \Delta \, \partial \mathcal{H}(\mathbf{0}) .$$

Now from the expression of $E_n^{(2)}$:

$$E_n^{(2)} = \frac{\gamma}{9} \sum_{n' (\neq n)} \frac{| \langle n | V_{1/2} | n' \rangle |^2}{2 \omega (n - n')}$$

where only $n' = n \pm 1$ and $n \pm 3$ contribute, one deduces :

$$E_n^{(2)} = \frac{-\gamma}{144\,\omega} [9(3n^2 + 3n + 1) \,.\, |\Delta\, \partial \mathcal{K}(\mathbf{0})|^2 + (3n^2 + 3n + 2) \,.\, |\partial^3 \mathcal{K}(\mathbf{0})|^2] \,. \quad (3.24)$$

The desired result is a direct consequence of equations (3.23) and (3.24) :

$$E_n = \mathcal{K}(\mathbf{0}) + \frac{\gamma}{2} [(2n + 1)\,\omega + E_n^{(1)} + E_n^{(2)} + 0(\gamma^2)] \,. \quad (3.25)$$

c) *Remarks.* — Regarding the obtained result, three remarks are of order.

i) For a large class of 2D lattices, the symmetry property : $\mathcal{K}(-\mathbf{k}) = \mathcal{K}(\mathbf{k})$ holds. In this case, $E_n^{(2)} = 0$.

ii) Equation (3.19) remains true, even if the classical version of the Hamiltonian has an explicit dependence on γ.

iii) In the expansion of E_n, one remarks the absence of terms in $0(\gamma^{1/2})$, $0(\gamma^{3/2})$, etc. This general property follows from the fact that H can always be written as : $H = \mathcal{K}(\mathbf{0}, 0) + \gamma \,.\, h$ with $h = h_0 + \gamma^{1/2} W_{1/2} + \gamma W_1 + 0(\gamma^{3/2})$. Here, h_0 is the harmonic oscillator part which gives the first order term $0(\gamma)$. To order γ^2, the property $\langle n | W_{1/2} | n \rangle = 0$ eliminates the diagonal contribution of $W_{1/2}$, and this because $W_{1/2}$ is odd in the K's. The only remaining contribution is the non-diagonal term $|\langle n | W_{1/2} | n' \rangle|^2$ as shown before.

3.4 HIGH ORDER EXPANSION. — We outline here the systematic expansion of E_n in the case of Harper's problem. With obvious notations, we have :

$$\begin{aligned} H &= 4 - 2\cos(\gamma^{1/2} K_1) - 2\cos(\gamma^{1/2} K^2) \\ &= \gamma(H_0 + V) + 0(\gamma^4) \end{aligned}$$

where : $$H_0 = K_1^2 + K_2^2, \quad V = -\frac{\gamma}{12}(K_1^4 + K_2^4) + \frac{2\gamma^2}{6!}(K_1^6 + K_2^6) \,. \quad (3.26)$$

The eigenvalues are given by :

$$e_n = \gamma \left[(2n + 1) + \langle n | V | n \rangle + \sum_{\ell (\neq n)} \frac{|\langle n | V | \ell \rangle|^2}{2(n - \ell)} + 0(V^3) \right] . \quad (3.27)$$

The required matrix elements are :

$$J_1 \equiv -\frac{\gamma^2}{12} \langle n | (K_1^4 + K_2^4) | n \rangle + \frac{2\gamma^3}{6!} \langle n | (K_1^6 + K_2^6) | n \rangle$$

and $$J_2 \equiv \frac{\gamma}{2} \sum_{\ell (\neq n)} \frac{\left| \langle n | \frac{\gamma}{12} (K_1^4 + K_2^4) | \ell \rangle \right|^2}{n - \ell} \,.$$

Explicit calculations of J_1 and J_2 are outlined in Appendix A. In particular,

$$2\langle n | \frac{K_1^4 + K_2^4}{4!} | n \rangle = \frac{1}{16} [1 + (1 + 2n)^2] \,,$$

$$2\langle n | \frac{K_1^6 + K_2^6}{6!} | n \rangle = \frac{1}{9 \times 32} (4n^3 + 6n^2 + 8n + 3) \,,$$

and $$J_2 = -\frac{\gamma^3}{32 \times 144} [(n + 1)(n + 2)(n + 3)(n + 4) - n(n - 1)(n - 2)(n - 3)] \,.$$

This leads to the following result :

$$e_n = \gamma(2n+1) - \frac{\gamma^2}{16}[1 + (1+2n)^2] + \frac{\gamma^3}{64 \times 3}[n^3 + (n+1)^3] + 0(\gamma^4) . \quad (3.28)$$

3.5 TWO EXAMPLES. — a) *Simple square lattice.* — With appropriate notations, one has $\mathcal{H}(\mathbf{k}) = -2\cos k_1 - 2\cos k_2$. The critical point is $\mathbf{k}_c = (0, 0)$ and then : $\mathcal{H}(\mathbf{0}) = -4$, $\partial^2\mathcal{H}(\mathbf{0}) = 2 . \mathbb{1}$, $\omega = 2$ and $\Delta^2\mathcal{H}(\mathbf{0}) = -4$. In this case (Eq. (3.13)) reduces to equation (3.11) as it should be.

b) *Two flux triangular lattice.* — Using equation (2.41), $\mathcal{H}(\mathbf{k})$ exhibits an explicit dependence on the flux :

$$\mathcal{H}(\mathbf{k}) = 2\cos k_1 + 2\cos k_2 + 2\cos\left(k_1 + k_2 + \frac{\gamma}{2} - \eta\right) , \quad (3.29)$$

We consider first the critical points at $\gamma = 0$. One has :

— Saddle points : $k_1 = k_2 = \pi + \eta$; $k_1 = -\eta$, $k_2 = \pi + \eta$ and $k_1 = \pi + \eta$, $k_2 = -\eta$.

— Minima or maxima : occurring at points P of coordinates $k_1 = k_2 = \frac{2\pi}{3}\varepsilon + \frac{\eta}{3} \equiv \theta_\varepsilon$ with $\varepsilon = -1$, 0 or 1. At this point, $\mathcal{H}(P) = 6\cos\theta$ and $\partial^2\mathcal{H}(P) = -2\cos\theta \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$. Thus, P corresponds to a maximum (resp. minimum) if $\cos\theta_\varepsilon > 0$ (resp. $\cos\theta_\varepsilon < 0$) and to a singular point if $\cos\theta_\varepsilon = 0$.

An appropriate change of coordinates, $k_{1,2} = \frac{1}{\sqrt{2}}(3^{-1/4}\hat{k}_1 \pm 3^{-1/4}\hat{k}_2)$, reduces $\mathcal{H}(\mathbf{k})$ near P to :

$$\mathcal{H}(\mathbf{k}) = \sum_{\ell=1} 2\cos(\theta + \langle \hat{k} | \hat{e}_\ell \rangle) , \quad (3.30)$$

where

$$\hat{e}_1 = \left(\frac{2}{\sqrt{3}}\right)^{1/2}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) , \quad \hat{e}_2 = \left(\frac{2}{\sqrt{3}}\right)^{1/2}\left(\frac{1}{2}, \frac{-\sqrt{3}}{2}\right) ,$$

$$\hat{e}_3 = \left(\frac{2}{\sqrt{3}}\right)^{1/2}(-1, 0) .$$

In this new frame $(\hat{k}_1, \hat{k}_2)$, the matrix of second derivatives becomes a scalar one. The quantization of $\mathcal{H}$ can then performed as usual : $\hat{k}_\mu \to \gamma^{1/2} K_\mu$, with $[K_1, K_2] = i$.

For weak γ, H reduces to :

$$H = 6\cos\theta - \gamma\sqrt{3}\cos\theta . (K_1^2 + K_2^2) + \gamma^{3/2}\frac{\sin\theta}{3^{3/4}2^{1/2}} \times$$

$$\times (-K_1^3 + 3K_2K_1K_2) + \gamma^2\frac{\cos\theta}{8}[1 + (K_1^2 + K_2^2)^2] + 0(\gamma^{5/2}) . \quad (3.31)$$

The expansion of the eingenvalues in powers of γ is immediate. Only the term $0(\gamma^{3/2})$ has to be treated as a second order perturbation of the remaining diagonal terms. The result is :

$$E_n = 6\cos\theta - \gamma\sqrt{3}\cos\theta . (2n+1) + \frac{\gamma^2}{8}[1 + (1+2n)^2] \times$$

$$\times \cos\theta + \frac{\gamma^2}{18}\frac{\sin^2\theta}{\cos\theta}\left[\frac{3(2n+1)^2 + 5}{4}\right] . \quad (3.32)$$

This expression of E_n is identical to that predicted by equation (3.13). Indeed, in the present case, we have respectively : $\mathcal{K}(\mathbf{0}) = 6\cos\theta$, $\partial\mathcal{K}(\mathbf{0}) = 0$, $\Delta\mathcal{K}(\mathbf{0}) = 2\omega = -4\cos\theta \cdot \sqrt{3}$, $\Delta^2\mathcal{K}(\mathbf{0}) = 8\cos\theta$, $\Delta\,\partial\mathcal{K}(\mathbf{0}) = 0$ and $\partial^3\mathcal{K}(\mathbf{0}) = -2^{5/3}3^{1/4}\sin\theta$. Notice that $E_n^{(2)} \neq 0$ is this example (lack of inversion center symmetry). Furthermore, the above formula does not work at the singular point $\cos\theta = 0$ because $\omega = 0$ and H assumes a singular form : $H = \frac{\gamma^{3/2}}{3^3 2^{1/2}}(3K_2K_1K_2 - K_1^3) + 0(\gamma^{5/2})$.

4. Semi-Classical Expansion at Rational Magnetic Flux.

During several years, the possible extension of semi-classical ideas to rational flux remained without solution [14]. The first successful attempts [10, 11] are very recent and limited to specific examples. To our knowledge the first general formulation of this problem has been given by one of us [7] (see also Ref. [12]), within the algebraic formalism depicted in section 2. In this section, we outline a systematic semi-classical expansion near rational flux. This line of approach is original, and leads to new results not derived before.

4.1 QUANTIZATION METHOD. — The method of quantization is based on a weak version of the renormalization group methodology. The idea is that whenever α is close to a rational number p/q, the rotation algebra $\mathcal{A}(\alpha)$ can be identified with the subalgebra of $M_q \otimes \mathcal{A}\left(\alpha - \frac{p}{q}\right)$ generated by the elements :

$$U_\alpha = W_1 \otimes U_{\alpha - p/q}, \quad V_\alpha = W_2 \otimes V_{\alpha - p/q} \tag{4.1}$$

where W_1 and W_2 are two $q \times q$ unitary matrix such that $W_1 W_2 = e^{2i\pi p/q} W_2 W_1$ and $W_1^q = W_2^q = \mathbb{1}$.

Using this representation, one can write the Hamiltonian as a matrix with entries in $\mathcal{A}\left(\alpha - \frac{p}{q}\right)$. For $\alpha = p/q$, the entries become functions of the variable $\mathbf{k}$. Therefore, the spectrum can be computed simply by diagonalizing the corresponding matrix for each $\mathbf{k}$, giving rise to band spectrum. For α very close to p/q, the gaps and bands structure is maintained. This allows in particular the possibility of defining bands. For the sake of clarity, we consider a non degenerate band B. This means that if P denotes the eigenprojection of the band at the value $\alpha = p/q$, then $\mathrm{tr}P(\mathbf{k}) = 1$ for all $\mathbf{k}$'s. In what follows, we show how to use this formulation.

Let tr_q represents the partial trace induced by the usual trace on the algebra M_q on $M_q \otimes \mathcal{A}(\alpha - p/q)$. Under these conditions, one can show that, up to a correction of order $0((\alpha - p/q)^2)$, the lower $E(\alpha)$ (resp. the upper) edge of the band B, is identical to $E'(\alpha)$ which is the lower (resp. the upper) edge of the spectrum of the element $\mathrm{tr}_q(H_B)$ of $\mathcal{A}(\alpha - p/q)$. As a consequence, the so-called Wilkinson-Rammal formula results : The lower (resp. the upper) edge of the band $E^-(\alpha)$ (resp. $E^+(\alpha)$) of a non degenerate band of H at $\alpha = p/q$ is given by :

$$E^\pm(\alpha) = E^\pm(p/q) - (\pm)\, a\left|\alpha - \frac{p}{q}\right| + b\left(\alpha - \frac{p}{q}\right) + 0\left(\left|\alpha - \frac{p}{q}\right|^{3/2}\right) \tag{4.2}$$

with

$$a = 2\pi q^2 \Big/ \rho\left(E^\pm\left(\frac{p}{q}\right)\right) \tag{4.3}$$

and

$$b = \frac{1}{4\,i\pi}\,\mathrm{tr}_q\,\{P(\mathbf{k})\,.\,(\partial_1 H(\mathbf{k})\,.\,\partial_2 P(\mathbf{k}) - \partial_2 H(\mathbf{k})\,.\,\partial_1 P(\mathbf{k}))\}_{E_B(\mathbf{k}) = E^{\pm}(p/q)}\,. \tag{4.4}$$

This by now well known formula contains three contributions. The first term is the value of the energy at the band edge for $\alpha = p/q$. The second represents a standard harmonic oscillator part. The occurrence of the density of states $\rho(E_B(\mathbf{0}))$ is due to the following observation. The element $\mathrm{tr}_q(H_B)$ of $\mathcal{A}(\alpha - p/q)$ coincides at $\alpha = p/q$ with the band energy function $E_B(\mathbf{k})$. If we now apply (Eq. (3.2)) to $\mathrm{tr}_q(H_B)$ we need first to compute the matrix of second derivatives of $E_B(\mathbf{k})$ at the bottom (resp. the top) of the band. However, the determinant $\det^{1/2}\left(\frac{1}{2}\,\partial_\mu\,\partial_\nu E_B(\mathbf{0})\right)$ is nothing but q^2 time the inverse of the local density of states $\rho(E_B(\mathbf{0}))$ at the corresponding band edge. The last term in equation (4.2) comes from Berry's phase [10, 20], namely from the fact that the eigenprojection $P(\mathbf{k})$ at the value $\alpha = p/q$ defines in general a non trivial line bundle over the 2-torus (k_1, k_2). Notice that this new term is *not* the Chern class of the bundle for the Chern class is obtained firstly in dividing the trace by q, replacing H by P in equation (4.4) and then integrating over the 2-torus (Brillouin zone). Here, we do not integrate, but we rather evaluate the integrand at the band edge.

The above formula corresponds to the first order semi-classical expansion, and has been established for an element H such that $\partial H = 0$. If $\partial H \neq 0$, there is an additional contribution to the second term which is easy to compute (analogous to $\alpha\,\frac{\partial H}{\partial \alpha}$ in Eq. (3.2)). A new derivation of the formula (Eq. (4.2)) will be given below, within a systematic expansion in $\gamma = 2\,\pi\,(\alpha - p/q)$. For practical purposes a possible choice for the two $q \times q$ matrices W_1 and W_2 is the following one: W_1 is a diagonal matrix, with elements $(W_1)_{\ell,\ell} = \exp\left(2\,i\,\pi\,\frac{p}{q}\cdot\ell\right)$, $1 \leqslant \ell \leqslant q$; $(W_2)_{\ell;\ell+1} = 1$, $1 \leqslant \ell \leqslant q-1$ and $(W_2)_{q,1} = 1$. This choice satisfies trivially the required conditions: $W_1^q = W_2^q = \mathbb{1}$ and $W_1\,W_2 = \mathrm{e}^{-2\,i\pi p/q}\,W_2\,W_1$.

4.2 SIMPLE EXAMPLE. — Before considering the general case, let us work out a warming up example: Harper equation at $p/q = 1/2$. In this case:

$$W_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \sigma_3\,, \quad W_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \sigma_1 \tag{4.5}$$

where σ_1, σ_2 and σ_3 are Pauli matrices $\left(\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\right)$.

Following the method described above, the original Hamiltonian $H = U + V + \mathrm{h.c.}$ is transformed first into:

$$H = (\mathrm{e}^{ik_2}\,W_2 + \mathrm{e}^{ik_1}\,W_1) + \mathrm{h.c.} \tag{4.6}$$

by using $U \to \mathrm{e}^{ik_2}\,W_2$ and $V \to \mathrm{e}^{ik_1}\,W_1$.

The quantized of H is obtained as usual. For a critical point located at $\mathbf{k} = 0$, one replaces k_μ by $\gamma^{1/2} K_\mu$ and this implies:

$$H = 2\cos\,(\gamma^{1/2} K_1)\,.\,\sigma_3 + 2\cos\,(\gamma^{1/2}\,.\,K_2)\,.\,\sigma_1\,. \tag{4.7}$$

Before quantization, the band structure is given by two subbands: $\varepsilon = \pm\,2(\cos^2 k_1 + \cos^2 k_2)^{1/2}$ which degenerate at $\varepsilon = 0$. In what follows, we consider the semi-classical expansion near $\varepsilon = \pm\,2\,\sqrt{2}$ and $\varepsilon = 0$ respectively.

a) $\varepsilon = \pm 2\sqrt{2}$. — This energy is reached at the critical point $k_1 = k_2 = 0$. Instead of expanding H as given by equation (4.7), in powers of γ, it is more convenient to consider H^2:

$$H^2 = 2(1 + \cos 2\gamma^{1/2} K_1) + 2(1 + \cos 2\gamma^{1/2} K_2) + \\ + 4i\sigma_2(\cos \gamma^{1/2} K_1 \,.\, \cos \gamma^{1/2} K_2 - \cos \gamma^{1/2} K_2 \,.\, \cos \gamma^{1/2} K_1) \,. \quad (4.8)$$

Expanding equation (4.8), up to order γ^2, one obtains:

$$H^2 = 8 - 4\gamma(K_1^2 + K_2^2) + \frac{2^5}{24}\gamma^2(K_1^4 + K_2^4) - 4\gamma^2\sigma_2 \,.\, (K_1 K_2 + K_2 K_1) + 0(\gamma^4) \,.$$

Using: $\langle n | K_\mu^2 | n \rangle = \frac{3}{8}(1 + (1 + 2n)^2)$, $\langle n | K_1 K_2 | n \rangle = i/2$, one deduces:

$$E_n^2 = 8 - 4\gamma(2n + 1) + \gamma^2(1 + (1 + 2n)^2) \quad (4.9)$$

which describes the Landau levels near the band edge $\varepsilon = \pm 2\sqrt{2}$.

b) $\varepsilon = 0$ (*see Ref.* [12]). — This critical value is reached at $k_1 = k_2 = \pi/2$. Therefore, the quantization rule is: $k_\mu \to \frac{\pi}{2} + \gamma^{1/2} K_\mu$ and then

$$-H = 2\sin(\gamma^{1/2} K_1) \,.\, \sigma_3 + 2\sin(\gamma^{1/2} K_2) \,.\, \sigma_1 \,. \quad (4.10)$$

To first order in γ, one obtains: $-H = 2\gamma^{1/2}(K_1 \,.\, \sigma_3 + K_2 \,.\, \sigma_1)$. This Hamiltonian can be simply diagonalized, because of its equivalence with Dirac Hamiltonian:

$$H_0 = \begin{pmatrix} K_1 & K_2 \\ K_2 & -K_1 \end{pmatrix} \approx \begin{pmatrix} 0 & K_1 - iK_2 \\ K_1 + iK_2 & 0 \end{pmatrix}$$

and then $H_0^2 = K_1^2 + K_2^2 + i\sigma_2[K_1, K_2] = K_1^2 + K_2^2 - \sigma_3 \,.$

The eigenvalues are: $2n$ and $2(n + 1)$ and then $E_n = \pm (8n\gamma)^{1/2}$. To the next order in γ, H is expanded further as:

$$-H = 2\gamma^{1/2}\left\{\left(K_1 - \frac{\gamma}{6}K_1^3\right) \cdot \sigma_3 + \left(K_2 - \frac{\gamma}{6}K_2^3\right) \cdot \sigma_1\right\} \,. \quad (4.11)$$

The perturbation calculation, performed on H^2 leads to the final result

$$E_n^2 = 4\gamma\left[(2n + 1) \pm 1 - \frac{\gamma}{4}((2n + 1)^2 + 1) \pm \frac{1}{2}\gamma(2n + 1)\right]$$

i.e.

$$E_n = \pm 2(2n\gamma)^{1/2}\left(1 - \frac{\gamma n}{2}\right)^{1/2} \,. \quad (4.12)$$

4.3 GENERAL CASE. — The semi-classical expansion at arbitrary p/q is based on the so-called Schur formula [21]. Let $H = H^*$ be a self-adjoint operator, acting on a Hilbert space $\mathfrak{H} \oplus \mathfrak{Q}$, and E be an eigenvalue of H. If P (resp. Q) is the eigenprojector on subspace $\mathfrak{H}$ (resp. $\mathfrak{Q}$), then each E not in the spectrum of QHQ, is also eigenvalue of the effective Hamiltonian:

$$H_{\text{eff}}(E) = PHP + PHQ \,.\, (E - QHQ)^{-1} \,.\, QHP \quad (4.13)$$

H_{eff} describes the effective (or renormalized) Hamiltonian on $\mathfrak{P}$, where the eventual influence of $\mathfrak{Q}$ has been taken into account.

Of main interest for us is the case where $P = |\psi\rangle\langle\psi|$, i.e. of rank equal to one. In such a case $H_{\text{eff}}(E)$ reduces to a 1×1 matrix, i.e. to a scalar :

$$E = \langle\psi|H_{\text{eff}}(E)|\psi\rangle = \langle\psi|H|\psi\rangle + \langle\psi|HQ\frac{1}{E-QHQ}QH|\psi\rangle . \tag{4.14}$$

This is the fundamental equation to be used below. In this respect, we mention the following useful remark : if $Q = \sum_r |\psi_r\rangle\langle\psi_r|$ and $H|\psi_r\rangle = E_r|\psi_r\rangle$, then

$$(E-QHQ)^{-1} = \sum_r |\psi_r\rangle . (E-E_r)^{-1} . \langle\psi_r| . \tag{4.15}$$

We consider now a self-adjoint $q \times q$ matrix $\mathcal{K}(\mathbf{k})$, regular in $\mathbf{k} = (k_1, k_2)$. In the vicinity of $\mathbf{k} = 0$, we expand $\mathcal{K}(\mathbf{k})$ up to fourth order :

$$\mathcal{K}(\mathbf{k}) = \mathcal{K}(\mathbf{0}) + \partial_\mu\mathcal{K}(\mathbf{0}) . k_\mu + \frac{1}{2!}\partial_\mu\partial_\nu\mathcal{K}(\mathbf{0}) . k_\mu k_\nu + \frac{1}{3!}\partial_\mu\partial_\nu\partial_\rho\mathcal{K}(\mathbf{0}) . k_\mu k_\nu k_\rho + \\ + \frac{1}{4!}\partial_\mu\partial_\nu\partial_\rho\partial_\sigma\mathcal{K}(\mathbf{0}) . k_\mu k_\nu k_\rho k_\sigma + 0(k^5) . \tag{4.16}$$

Assume now that for $\mathbf{k} \simeq 0$, $\mathcal{K}(\mathbf{k})$ has the eigenvalues $e_1(\mathbf{k}), \ldots, e_q(\mathbf{k})$ with the corresponding eigenvectors $|1\rangle_k, \ldots, |q\rangle_k$. In the following, we will use the following notations :

$$P_s(k) = |s\rangle_{kk}\langle s| ; \quad P_s = P_s(0) \quad \text{and} \quad |\ell\rangle = |\ell\rangle_k \quad \text{at } \mathbf{k} = \mathbf{0} .$$

Similarly, we define : $\partial_{\mu_1} \ldots \partial_{\mu_s} e_\ell = \dfrac{\partial}{\partial k_{\mu_1}} \cdots \dfrac{\partial}{\partial k_{\mu_s}} e_\ell \Big|_{k=0}$, etc.

The purpose of the present section is the expansion of a generic eigenvalue $e_\ell(\mathbf{k})$ in powers of γ. For this we assume that $e_\ell(\mathbf{k})$ is non degenerate at $\mathbf{k} \sim \mathbf{0}$, and :

$$e_\ell(\mathbf{k}) = e_\ell + \frac{\omega}{2}(k_1^2 + k_2^2) + 0(|k|^3) , \quad k \sim \mathbf{0} , \quad \omega \neq 0 . \tag{4.17}$$

This assumption means that $\mathbf{k} = 0$ is a regular minima or maxima of e_ℓ and the matrix of second derivatives $\partial_\mu\partial_\nu e$ is scalar. Unless very exceptional cases, one can always find local coordinates such that equation (4.17) is fulfilled. The normal form of $e_\ell(\mathbf{k})$ allows for a natural quantization procedure (Weyl quantization) : $k_\mu \to \gamma^{1/2}K_\mu$, where K_μ are two self-adjoint operators, such that $[K_1, K_2] = i$. The quantized of $\mathcal{K}$ is a matrix valued operator :

$$H = \mathcal{K}(\mathbf{0}) + \gamma^{1/2}\partial_\mu\mathcal{K}(\mathbf{0}) . K_\mu + \frac{\gamma}{2!}\partial_\mu\partial_\nu\mathcal{K}(\mathbf{0}) . K_\mu K_\nu + \frac{\gamma^{3/2}}{3!}\partial_\mu\partial_\nu\partial_\rho\mathcal{K}(\mathbf{0}) . K_\mu K_\nu K_\rho + \\ + \frac{\gamma^2}{4!}\partial_\mu\partial_\nu\partial_\rho\partial_\sigma\mathcal{K}(\mathbf{0}) . K_\mu K_\nu K_\rho K_\sigma + 0(\gamma^{5/2}) . \tag{4.18}$$

a) *First order* $0(\gamma)$ *calculation.* — Our aim here is to get a quantized operator $E_\ell = e_\ell + 0(\gamma)$ by diagonalizing the matrix H and then deduce an expansion in γ of the harmonic oscillator type

$$E_\ell = e_\ell + \sigma . \gamma + \gamma\frac{\omega}{2}(K_1^2 + K_2^2) . \tag{4.19}$$

For this we use Schur formula (Eq. (4.14)) :

$$E_\ell = \langle \ell | H | \ell \rangle + \langle \ell | HQ \,.\, (E_\ell - QHQ)^{-1} \,.\, QH | \ell \rangle \,. \tag{4.20}$$

Remember that E_ℓ is a scalar operator, depending on K's and $Q = \mathbb{1} - |\ell\rangle\langle\ell|$. Giving that $\mathcal{H} \equiv \mathcal{H}(\mathbf{0})$ is a diagonal matrix in the basis $|1\rangle, \ldots, |q\rangle$ and K_μ commutes with the matrix elements of $\mathcal{H}(\mathbf{k})$, it follows that

$$\begin{aligned} QH|\ell\rangle &= Q\left(\mathcal{H} + \gamma^{1/2} \,.\, \partial_\mu \mathcal{H} \,.\, K_\mu + \frac{\gamma}{2!}\, \partial_\mu\, \partial_\nu \mathcal{H} \,.\, K_\mu\, K_\nu + \cdots\right) |\ell\rangle \\ &= \gamma^{1/2} \,.\, Q\, \partial_\mu \mathcal{H} \,.\, |\ell\rangle \,.\, K_\mu + \frac{\gamma}{2!}\, Q\, \partial_\mu\, \partial_\nu \mathcal{H} \,.\, |\ell\rangle \,.\, K_\mu\, K_\nu + 0(\gamma^{3/2}) \\ &= 0(\gamma^{1/2}) \end{aligned}$$

and then

$$\begin{aligned} E_\ell &= \langle \ell | H | \ell \rangle + 0(\gamma) \\ &= e_\ell + \gamma^{1/2} \langle \ell | \partial_\mu \mathcal{H} | \ell \rangle \,.\, K_\mu + \frac{\gamma}{2} \langle \ell | \partial_\mu\, \delta_\nu \mathcal{H} | \ell \rangle \,.\, K_\mu\, K_\nu + 0(\gamma) \,. \end{aligned}$$

Using Feynmann-Hellman theorem, one deduces :

$$\langle \ell | \partial_\mu \mathcal{H} | \ell \rangle / \langle \ell | \ell \rangle = \partial_\mu e_\ell = 0$$

and then

$$E_\ell = e_\ell + 0(\gamma) \,. \tag{4.21}$$

This zero order approximation for E_ℓ, has to be used as initial value in the iteration scheme prescribed by equation (4.20). This leads to :

$$E_\ell = e_\ell + \frac{\gamma}{2} \langle \ell | \partial_\mu\, \partial_\nu \mathcal{H} | \ell \rangle \cdot K_\mu\, K_\nu + \gamma \cdot \langle \ell | \partial_\nu \mathcal{H} \cdot Q \cdot \frac{1}{e_\ell - QHQ + 0\,(\gamma^{1/2})}\, Q\, \partial_\mu \mathcal{H} | \ell \rangle \times \\ \times K_\mu\, K_\nu + 0(\gamma^{3/2}) \,.$$

Following equation (4.15), this can also be written as :

$$E_\ell = e_\ell + \left[\frac{\gamma}{2} \langle \ell | \partial_\mu\, \partial_\nu \mathcal{H} | \ell \rangle + \gamma \sum_{\ell' (\neq \ell)} \frac{\langle \ell | \partial_\mu \mathcal{H} | \ell' \rangle \langle \ell' | \partial_\nu \mathcal{H} | \ell \rangle}{e_\ell - e_{\ell'}} \right] K_\mu\, K_\nu + 0(\gamma^{3/2})$$

i.e.

$$E_\ell \equiv e_\ell + \gamma \,.\, R^{(2)}_{\mu\nu} K_\mu\, K_\nu + 0(\gamma^{3/2}) \,.$$

The tensor $R^{(2)}_{\mu\nu}$ so defined can be decomposed as follows :

$$R^{(2)}_{\mu\nu} K_\mu\, K_\nu = \tilde{R}^{(2)}_{\mu\nu} K_\mu\, K_\nu + \frac{i}{2} (R^{(2)}_{12} - R^{(2)}_{21}) \,.$$

The symmetric part $\tilde{R}^{(2)}_{\mu\nu}$ can actually be identified as : $\tilde{R}^{(2)}_{\mu\nu} = \dfrac{\omega}{2}\, \delta_{\mu\nu}$, whereas the remaining antisymmetric part is given by : $\sigma = \dfrac{i}{2} (R^{(2)}_{12} - R^{(2)}_{21})$. This new term σ is a Berry's phase term, given explicitely as :

$$\sigma = \frac{i}{2} \sum_{\ell' (\neq \ell)} \frac{\langle \ell | \partial_1 \mathcal{H} | \ell' \rangle \langle \ell' | \partial_2 \mathcal{H} | \ell \rangle - \langle \ell | \partial_2 \mathcal{H} | \ell' \rangle \langle \ell' | \partial_1 \mathcal{H} | \ell \rangle}{e_\ell - e_{\ell'}} \,. \tag{4.22}$$

Notice that an appropriate use of equation (C1) (Appendix C) leads to a simple expression for σ:

$$\sigma = \frac{i}{2} \left(\langle \ell | \partial_1 P_\ell \,.\, \partial_2 \mathcal{H} | \ell \rangle - \langle \ell | \partial_2 P_\ell \,.\, \partial_1 \mathcal{H} | \ell \rangle \right). \tag{4.23}$$

Further simplifications occur if $\partial_\mu e_\ell = 0$ is used for instance (see Eq. (4.38)). Therefore, the final result at order $0(\gamma)$ is given by

$$E_\ell = e_\ell + \gamma \frac{\omega}{2} (K_1^2 + K_2^2) + \sigma \,.\, \gamma + 0 (\gamma^{3/2}) \tag{4.24}$$

which is nothing else than the Wilkinson-Rammal formula (Eq. (4.2)).

b) *Next orders* $0(\gamma^{3/2})$ *and* $0(\gamma^2)$. — With equation (4.24) as entry, one can iterate equation (4.14) and get the next order $0(\gamma^{3/2})$ term:

$$E_\ell = e_\ell + \gamma \frac{\omega}{2} (K_1^2 + K_2^2) + \sigma\gamma + \frac{\gamma^{3/2}}{3!} (\partial_\mu \partial_\nu \partial_\rho e_\ell \,.\, K_\mu K_\nu K_\rho) + \\ + i\gamma^{3/2} (R^{(3)}_{1\mu 2} - R^{(3)}_{2\mu 1}) K_\mu \,. \tag{4.25}$$

Here we have defined the tensor $R^{(3)}_{\mu\nu\rho}$ given explicitely in Appendix B. Using the results of Appendix C, one can reduce the new term (third order Berry's like phase):

$$\sigma^{(3)}_\mu \equiv i (R^{(3)}_{1\mu 2} - R^{(3)}_{2\mu 1})$$

into a simpler form:

$$\sigma^{(3)}_\mu = \frac{i}{2} \langle \ell | [\partial_1 P_\ell, \partial_\mu \partial_2 \mathcal{H}] - [\partial_2 P_\ell, \partial_\mu \partial_1 \mathcal{H}] | \ell \rangle - \\ - i \langle \ell | \partial_1 P_\ell \,.\, \partial_\mu \mathcal{H} \,.\, \partial_2 P_\ell - \partial_2 P_\ell \,.\, \partial_\mu \mathcal{H} \,.\, \partial_1 P_\ell | \ell \rangle \,. \tag{4.26}$$

The next order $0(\gamma^2)$ term can be calculated similarly. The final result reads:

$$\gamma^2 [R^{(4)}_{\mu\nu\rho\sigma} K_\mu K_\nu K_\rho K_\sigma + \hat{R}^{(4)}_{\mu\nu} K_\mu K_\nu] \,, \tag{4.27}$$

where the new tensors are given in Appendix B. As before, further simplification can be done:

$$\hat{R}^{(4)}_{\mu\nu} K_\mu K_\nu = \sigma \langle \ell | \partial_1 P_\ell \,.\, \partial_2 P_\ell + \partial_2 P_\ell \,.\, \partial_1 P_\ell | \ell \rangle \frac{K_1 K_2 + K_2 K_1}{2} + i \frac{\sigma}{2} \langle \ell | [\partial_1 P_\ell, \partial_2 P_\ell] | \ell \rangle + \\ + \sigma \left\{ \langle \ell | \partial_1 P_\ell \,.\, \partial_1 P_\ell | \ell \rangle K_1^2 + \langle \ell | \partial_2 P_\ell \,.\, \partial_2 P_\ell | \ell \rangle \,.\, K_2^2 \right\} \tag{4.28}$$

$$R^{(4)}_{\mu\nu\rho\sigma} K_\mu K_\nu K_\rho K_\sigma = \frac{1}{24} \partial_\mu \partial_\nu \partial_\rho \partial_\sigma e_\ell \,.\, K_\mu K_\nu K_\rho K_\sigma + \check{R}^{(4)}_{\mu\nu} K_\mu K_\nu + \check{\check{R}}^{(4)} \,. \tag{4.29}$$

The last two terms in equation (4.29) are fourth order Berry's-like phases, and are given by:

$$\check{R}^{(4)}_{11} = \frac{i}{2} [3(R_{1112} - R_{2111}) + (R_{1121} - R_{1211})] \,,$$

$$\check{R}^{(4)}_{22} = \frac{i}{2} [3(R_{1222} - R_{2221}) + (R_{2122} - R_{2212})] \,,$$

$$\check{R}^{(4)}_{12} = \check{R}^{(4)}_{21} = \frac{i}{2} [2(R_{1122} - R_{2211}) + (R_{1212} - R_{2121})] \,,$$

$$\check{\check{R}}^{(4)} = \frac{1}{2} [R_{1221} + R_{2112} - R_{1122} - R_{2211}] \,.$$

To summarize, the operator E_ℓ reads at order γ^2:

$$E_\ell\ e_\ell + \gamma\,\frac{\omega}{2}\,(K_1^2 + K_2^2) + \sigma\,.\,\gamma + \frac{1}{6}\,\gamma^{3/2}(\partial_\mu\,\partial_\nu\,\partial_\rho\,e_\ell)\,K_\mu\,K_\nu\,K_\rho + \gamma^{3/2}\sigma_\mu^{(3)}\,K_\mu + \\ + \gamma^2[R^{(4)}_{\mu\nu\rho\sigma}\,K_\mu\,K_\nu\,K_\rho\,K_\sigma + \hat{R}^{(4)}_{\mu\nu}\,K_\mu\,K_\nu]. \quad (4.30)$$

c) *Energy levels.* — Equation (4.30) allows for an expansion of the Landau levels in powers of γ. One remarks first that $\check{R}^{(4)}_{12}$ and $\check{R}^{(4)}_{21}$ make no contribution to E_n. The other terms $\check{\check{R}}^{(4)}$, $\check{R}^{(4)}$ and $\hat{R}^{(4)}$ contribute to the first order whereas the contribution of $\sigma_\mu^{(3)}$ appears at the second order perturbation.

To first order in γ, we recovers the formula (4.2):

$$E_n = e_\ell + \sigma\gamma + \frac{\omega}{2}\,(2n+1)\,.\,|\gamma|\,, \quad n = 0, 1, 2, \ldots \quad (4.31)$$

The second order correction to equation (4.31) is the sum of two terms $\delta E_n^{(1)}$ and $\delta E_n^{(2)}$ given by:

$$\delta E_n^{(1)} = \frac{\gamma^2}{64}\,[1 + (1+2n)^2]\,.\,(\partial_1^2 + \partial_2^2)\,e_\ell + \gamma^2\,.\,\chi_\ell \quad (4.32)$$

$$\delta E_n^{(2)} = \frac{\gamma}{2}\left\{-\frac{\gamma}{144\,\omega}\,[9(3n^2+3n+1)\,.\,|\Delta\,\partial e|^2 + (3n^2+3n+2)\,|\partial^3 e|^2] - \right. \\ \left. - \frac{\gamma}{2\,\omega}\,(2n+1)[\sigma_1^{(3)}\,.\,\Delta\,\partial_1 e + \sigma_2^{(3)}\,.\,\Delta\,\partial_2 e] - \frac{\gamma}{\omega}\,[(\sigma_1^{(3)})^2 + (\sigma_2^{(3)})^2]\right\}. \quad (4.33)$$

In equation (4.32), we have used the notation:

$$\chi_\ell = \left[\check{\check{R}}^{(4)} + \frac{1}{2}\,(2n+1)(\check{R}^{(4)}_{11} + \check{R}^{(4)}_{22}) + \frac{i}{2}\,\sigma\,\langle\ell\,|\,[\partial_1 P, \partial_2 P]\,|\,\ell\rangle + \right. \\ \left. + \frac{\sigma}{2}\,(2n+1)\,.\,\langle\ell\,|\,\partial_1 P_\ell\,.\,\partial_1 P_\ell + \partial_2 P_\ell\,.\,\partial_2 P_\ell\,|\,\ell\rangle\right].$$

These new results have to be compared with the zero flux limit. The main difference is certainly the proliferation of Berry's phases: σ, $\sigma_\mu^{(3)}$, $\check{R}^{(4)}$, etc. This is a non trivial new feature, that is difficult to get from the standard WKB or the equation-of-motion methods [22]. Remember that all the results of this paper have been obtained without any reference to wave functions or eigenmodes. In this respect, this is a definitive advantage of the algebraic formalism in comparison with other methods. In principle, one can formally obtain an infinite series expansion of E_n *vs.* γ. Without performing such a calculation, such a series is certainly more complicated than that obtained by Berry [23] for a simpler problem.

4.4 COMPUTATIONAL ASPECTS, EXAMPLES. — In this section we illustrate the previous results on two examples. For the sake of clarity we limit our discussion to the first order expansion. As working example we consider Harper equation:

$$\mathcal{H}(\mathbf{k}) = (W_1\,e^{ik_1} + W_2\,e^{ik_2}) + \text{h.c.} \quad (4.34)$$

with

$$\left(\gamma_0 = 2\,\pi\,\frac{p}{q}\right) : W_1 = \begin{pmatrix} e^{i\gamma_0} & 0 \\ 0 & e^{iq\gamma_0} \end{pmatrix} \quad \text{and} \quad W_2 = \begin{pmatrix} 0 & 1 & & 0 \\ 0 & 0 & 1 & \\ & & & 1 \\ 1 & & & 0 \end{pmatrix}.$$

Unless accidental degeneracy, there is q subbands at each rational flux p/q, given by the dispersion relation [24] :

$$P_q(e) - 2(\cos qk_1 + \cos qk_2) = 0 \tag{4.35}$$

where $P_q(e) = e^q + \cdots$ is a polynomial of degree q in e. The band edges are given by $P_q(e) = \pm 4$ and correspond to the critical points (k_1, k_2) specified by : $\cos qk_1 = \cos qk_2 = \pm 1$. Unless special mention, we will assume $k_1 = k_2 = 0$. In the notations of the previous section, the eigenvectors $|\ell\rangle$ assume the following form :

$$\psi \equiv (\psi_1, \psi_2, ..., \psi_m, ..., \psi_q) \quad \text{with} \quad \psi_m = \psi_{q+m} .$$

To first order in γ, one has to calculate only two parameters : ω and σ. From the definition of ω and equation (4.35), one deduces immediately

$$\omega = -2q^2/P'_q(e) \tag{4.36}$$

where the derivative is taken at the subband edge of interest.

The computation of σ is not so immediate. We start from the expression (Eq. (4.23)) of σ :

$$\sigma = \frac{i}{2} \left(\langle \ell | \partial_1 P \cdot \partial_2 \mathcal{H} | \ell \rangle - \langle \ell | \partial_2 P \cdot \partial_1 \mathcal{H} | \ell \rangle \right) . \tag{4.37}$$

Using the property $\partial_\mu e = 0$, one can simplify σ as :

$$\begin{aligned} \sigma &= \frac{i}{2} \left[\left\langle \frac{\partial \psi}{\partial k_1} \middle| e - \mathcal{H} \middle| \frac{\partial \psi}{\partial k_2} \right\rangle - \left\langle \frac{\partial \psi}{\partial k_2} \middle| e - \mathcal{H} \middle| \frac{\partial \psi}{\partial k_1} \right\rangle \right] \\ &= \Im m \langle \partial_1 \psi | \mathcal{H} - e | \partial_2 \psi \rangle \end{aligned} \tag{4.38}$$

with $\mathcal{H}$ given by equation (4.34). The calculation of the last matrix element is a simple matter of eigenvectors computation. This can be performed for instance as follows. Define $(0 \leqslant \alpha, \beta \leqslant q+1)$ first $\Delta^{\alpha,\beta}$ as :

$$\Delta^{\alpha,\beta} = \det \begin{vmatrix} a_\alpha - e & u & 0 & & \\ & & & & \mathbf{0} \\ v & a_{\alpha+1} - e & u & & \\ & v & & & \\ \mathbf{0} & & & & \\ & & & & u \\ & & & v & a_\beta - e \end{vmatrix} \tag{4.39}$$

with the convention $\Delta^{1,0} \equiv 1$, $\Delta^{q,q-1} = 1$. Here, we used the notations $u = v^{-1} = e^{ik_2}$ and $a_m = 2\cos(k_1 + m\gamma_0)$. Solving $\mathcal{H}|\psi\rangle = e|\psi\rangle$ for ψ_m, leads to

$$\psi_m/\psi_q = (-1)^m \frac{\Delta^{m+1,q-1} v^m + (-1)^q u^{q-m} \Delta^{1,m-1}}{\Delta^{1,q-1}} , \quad m = 1, 2, ..., q-1 .$$

The definite solution is obtained, through fixing $\psi_q (\neq 0)$ by the normalization condition :

$$\sum_{m=1}^{q} |\psi_m|^2 = 1 .$$

This implies the following expression for $\sigma : \sigma = \mathcal{N}/\mathcal{D}$ with

$$\mathcal{N} = \sum_{m=1}^{q} 2 \sin (m\gamma_0)[\Delta^{1,q-(m+1)} + (-1)^q \Delta^{1,m-1}][-m\Delta^{1,q-(m+1)} + \\ + (-1)^q (q-m) \Delta^{1,m-1}]$$

and

$$\mathcal{D} = \sum_{m=1}^{q} [\Delta^{1,q-(m+1)} + (-1)^q \Delta^{1,m-1}]^2 . \tag{4.40}$$

A slightly different formula can be derived for the critical points $qk_1 = qk_2 = \pi$. Let us illustrate these formulae at simple rationals $p/q = 1/2$, $1/3$ and $1/4$. In the first case, close to $e = \pm 2\sqrt{2}$, one finds $\sigma = 0$ as it should be [10]. In the case $p/q = 1/3$, the upper edge of the spectrum is located as $e = 1 + \sqrt{3}$ and we find $\sigma = -1 + \frac{\sqrt{3}}{2}$ in agreement with reference [11]. Similarly at $p/q = 1/4$, we have $e = 2\sqrt{2}$ and equation (4.40) gives $\sigma = -\sqrt{2}/4$.

More complete results can be obtained at different band edges for fixed p/q. For instance at $p/q = 1/3$, we find ($P_3(e) = e^3 - 6e$) the following Landau level structures :

$$\text{at } e = 1 - \sqrt{3}: \qquad E_n = e + |\gamma| \frac{3}{4} (\sqrt{3}+1)(2n+1) + \gamma \left(1 + \frac{\sqrt{3}}{2}\right),$$

$$\text{at } e = -2: \qquad E_n = e - \frac{3}{2}(2n+1)|\gamma| + \sqrt{3}\,\gamma ,$$

$$\text{and finally at } e = 1 + \sqrt{3}: \; E_n = e - \frac{3}{4}(\sqrt{3}-1)(2n+1)|\gamma| + \left(\frac{\sqrt{3}}{2} - 1\right)\gamma .$$

We conclude this section with a non-trivial example, provided by the generalized square lattice (see Sect. 2.4 for notations). At zero magnetic field, the band structure is given by :

$$\mathcal{H}(\mathbf{k})/2t_1 = \cos k_1 + \cos k_2 + 2\mu \,.\cos k_1 \,.\cos k_2$$

where $\mu = t_2/t_1$. We limit our discussion to : $0 < \mu < 1/2$, $\mu_c = \pm 1/2$ being a « critical » value of μ. Taking $t_1 = 1$, the band edges are given by $e = \pm 4 - 4\mu$. Near the lower edge, the Landau levels are obtained from equation (3.13) as

$$E_n = -4(1+\mu) + |\gamma|(1+2\mu)(2n+1) - \frac{1}{16}(1+4\mu)[1 + (1+2n)^2]\,\gamma^2, \tag{4.41}$$

$$(\omega = 2(1+2\mu),\, \Delta^2\mathcal{H}(0) = -4(1+4\mu)) .$$

A more interesting situation occurs at $p/q = 1/2$, where $\mathcal{H}(\mathbf{k})$ assumes the form :

$$\mathcal{H} = \begin{pmatrix} a & b \\ b^* & -a \end{pmatrix}$$

with $a = 2\cos k_1$, $b = 2\cos k_2 + 4i\mu \,.\sin k_1 \sin k_2$. The dispersion equation $e^2 = a^2 + bb^*$ leads to two subbands, with a central gap $[-4\mu, 4\mu]$. Near the lower edge of the first subband (i.e. at $e = -\sqrt{8}$) which is reached at $k_1 = k_2 = 0$, one obtains : $\omega = \sqrt{2}$ and $\sigma = 0$. Thus, the cusp remains symmetric as for $\mu = 0$:

$$E_n = -\sqrt{8} + |\gamma| \frac{\sqrt{2}}{2}(2n+1) + 0(\gamma^2) .$$

The other edge of this lower subband ($e = 4\,\mu$) reached at $k_1 = k_2 = \pi/2$ exhibits a more interesting behavior : $\omega = (1 - 4\,\mu^2)/\mu$ and $\sigma = 1/2\,\mu$. Therefore,

$$E_n/4\,\mu = 1 - \frac{1 - 4\,\mu^2}{8\,\mu^2}(1 + 2n)|\gamma| + \frac{\gamma}{8\,\mu^2}. \tag{4.42}$$

This non trivial result must be compared with the singular behavior found at $\mu = 0$ (Eq. (4.12)) : $E_n = \pm (8\,n\gamma)^{1/2}\left(1 - \frac{\gamma n}{2}\right)^{1/2}$, which is clearly not the limit $\mu = 0$ of equation (4.42).

5. Concluding remarks.

In addition to the specific use [16] of the results derived in the present paper, the methodology we have used calls for some comments. This is probably the most concrete example where three ideas are simultaneously at work : Semiclassical calculation, renormalization group ideas and non commutative geometry. In this respect, it is very interesting to find other examples where these ideas can be applied. We believe that we have now a very powerful machinary which should be used in the cases where physical intuition is lacking. We quote just the case of Bloch electrons in a periodic magnetic field, where new results have been obtained recently by our group [25]. For more detailed discussions on the non commutative geometry and the semiclassical limit in quantum mechanics, we direct the reader to reference [26].

APPENDIX A

Useful matrix elements.

The low field expansion calls for the computation of some matrix elements of the simple harmonic oscillator. Using the standard notations : $K_1 = \frac{a + a^*}{2}$, $K_2 = \frac{a - a^*}{i\sqrt{2}}$, $[a, a^*] = 1$, we just illustrate a rather general procedure for the calculation of the appropriate matrix elements. For this we consider the case of $\langle n|K_\mu^{2r}|n\rangle$, r = integer. It is useful to introduce the generating function (η real) :

$$\varphi(\eta) = \langle n|\exp(i\eta K_1)|n\rangle\ . \tag{A1}$$

Using the commutation relation $[a, a^*] = 1$, and $|n\rangle = \frac{a^{*n}}{\sqrt{n!}}|0\rangle$, $\varphi(n)$ can be written as :

$$\varphi(\eta) = e^{-\eta^2/4}\langle n|e^{i\eta\frac{a^*}{\sqrt{2}}}e^{i\eta\frac{a}{\sqrt{2}}}|n\rangle = \frac{e^{-\eta^2/4}}{n!}\langle 0|e^{-i\eta a^*/\sqrt{2}}a^n e^{i\eta a^*/\sqrt{2}}a^{*n}e^{-i\eta a/\sqrt{2}}|0\rangle$$

$$= \frac{e^{-\eta^2/4}}{n!}\langle 0|\left(\mathbf{a} + \frac{i\eta}{\sqrt{2}}\right)^n\left(\mathbf{a}^* + \frac{i\eta}{\sqrt{2}}\right)^n|0\rangle\ . \tag{A2}$$

The expansion of each term in (A2) leads to :

$$\varphi(\eta) = \frac{e^{-\eta^2/4}}{n!}\sum_{m,m'\leqslant n}\binom{n}{m}\binom{n}{m'}\langle 0|\mathbf{a}^{n-m}\mathbf{a}^{*n-m}|0\rangle\ .\ i^{m+m'}\left(\frac{\eta}{\sqrt{2}}\right)^{m+m'}$$

$$= e^{-\eta^2/4}\sum_{m=0}\frac{n!}{(n-m)!}\frac{(-1)^m}{(m!)^2}\left(\frac{\eta^2}{2}\right)^m. \tag{A3}$$

Here we have used $\langle 0 | \mathbf{a}^{n-m}\, \mathbf{a}^{*n-m'} | 0 \rangle = \delta_{m,m'}(n-m)!$. $\varphi(\eta)$ can also be written as :

$$\varphi(\eta) = \sum_{m=0}^{n} \sum_{\ell=0}^{\infty} (-1)^{\ell+m} \frac{(\eta^2)^{\ell+m}}{2^{2m+2\ell}} \frac{n!}{(n-m)!\,(m!)^2\,\ell!}$$

$$= \sum_{\ell=0}^{\infty} \left(\frac{\eta^2}{2}\right)^r (-1)^r \sum_{m=0}^{n\wedge r} 2^{m-r} \frac{n!}{(n-m)!\,(m!)^2\,(r-m)!} \tag{A4}$$

$$\equiv \sum_{r=0}^{\infty} \frac{(-1)^r}{(2r)!} \langle n | K_1^{2r} | n \rangle \cdot \eta^{2r}. \tag{A5}$$

The comparison of (A4) and (A5) gives the desired result

$$\langle n | K_1^{2r+1} | n \rangle = 0\,,$$

$$\langle n | K_\mu^{2r} | n \rangle = 2^{-2r}(2r)! \sum_{m=0}^{n\wedge r} 2^m \frac{n!}{(n-m)!\,(m!)^2\,(r-m)!}\,. \tag{A6}$$

For instance, one obtains :

$$\langle n | K_1^2 + K_2^2 | n \rangle = 2n + 1$$

$$2\langle n | \frac{K_1^4 + K_2^4}{4!} | n \rangle = [1 + (1+2n)^2]/16$$

and finally

$$2\langle n | \frac{K_1^6 + K_2^6}{6!} | n \rangle = \frac{1}{32 \times 9}(3 + 8n + 6n^2 + 4n^3)\,. \tag{A7}$$

APPENDIX B

Second order expansion at rational flux.

In this Appendix we give the explicit expressions of the third and fourth order tensors used in the main text.

The third order tensor, which appear in equation (4.24) is given by :

$$R^{(3)}_{\mu\nu\rho} = \frac{1}{3!} \langle \ell | \partial_\mu\, \partial_\nu\, \partial_\rho \mathcal{H} | \ell \rangle +$$

$$+ \frac{1}{2} \sum_{\ell'(\neq \ell)} \frac{\langle \ell | \partial_\mu \mathcal{H} | \ell' \rangle \langle \ell' | \partial_\nu\, \partial_\rho \mathcal{H} | \ell \rangle + \langle \ell | \partial_\mu\, \partial_\nu \mathcal{H} | \ell' \rangle \langle \ell' | \partial_\rho \mathcal{H} | \ell \rangle}{e_\ell - e_{\ell'}}$$

$$+ \sum_{\ell', \ell''(\neq \ell)} \frac{\langle \ell | \partial_\mu \mathcal{H} | \ell' \rangle \langle \ell' | \partial_\nu \mathcal{H} | \ell'' \rangle \langle \ell'' | \partial_\rho \mathcal{H} | \ell \rangle}{(e_\ell - e_{\ell'})(e_\ell - e_{\ell''})}\,. \tag{B1}$$

Symmetry arguments can be used to show :

$$R^{(3)}_{\mu\nu\rho}\, K_\mu\, K_\nu\, K_\rho = (\partial_\mu\, \partial_\nu\, \partial_\rho \cdot e_\ell)\, K_\mu\, K_\nu\, K_\rho + iK_\mu (R^{(3)}_{1\mu 2} - R^{(3)}_{2\mu 1})\,. \tag{B2}$$

The other tensors appear in equation (4.27). The second is simply given by :

$$\hat{R}^{(4)}_{\mu\nu} = \sigma \cdot \sum_{\ell'(\neq \ell)} \frac{\langle \ell | \partial_\mu \mathcal{H} | \ell' \rangle \langle \ell' | \partial_\nu \mathcal{H} | \ell \rangle}{(e_\ell - e_{\ell'})^2} = \sigma \langle \ell | \partial_\mu P_\ell \cdot \partial_\nu P_\ell | \ell \rangle \tag{B3}$$

whereas the first is more involved :

$$
\begin{aligned}
R^{(4)}_{\mu\nu\rho\sigma} = {} & \frac{1}{24}\,\langle \ell \,|\, \partial_\mu\, \partial_\nu\, \partial_\rho\, \partial_\sigma \mathcal{H} \,|\, \ell \rangle \\
& + \frac{1}{4} \sum_{\ell' (\neq \ell)} \frac{\langle \ell \,|\, \partial_\mu\, \partial_\nu \mathcal{H} \,|\, \ell' \rangle \, \langle \ell' \,|\, \partial_\rho\, \partial_\sigma \mathcal{H} \,|\, \ell \rangle}{e_\ell - e_{\ell'}} \\
& + \frac{1}{2} \sum_{\ell', \ell'' (\neq \ell)} \left\{ \frac{\langle \ell \,|\, \partial_\mu \mathcal{H} \,|\, \ell' \rangle \, \langle \ell' \,|\, \partial_\nu \mathcal{H} \,|\, \ell'' \rangle \, \langle \ell'' \,|\, \partial_\rho\, \partial_\sigma \mathcal{H} \,|\, \ell \rangle}{(e_\ell - e_{\ell'})} \right. \\
& \left. + \frac{\langle \ell \,|\, \partial_\mu\, \partial_\nu \mathcal{H} \,|\, \ell' \rangle \, \langle \ell' \,|\, \partial_\rho \mathcal{H} \,|\, \ell'' \rangle \, \langle \ell'' \,|\, \partial_\sigma \mathcal{H} \,|\, \ell \rangle}{(e_\ell - e_{\ell'})(e_\ell - e_{\ell''})} \right\} \\
& + \frac{1}{2} \sum_{\substack{\ell', \ell'' \\ (\neq \ell)}} \frac{\langle \ell \,|\, \partial_\mu \mathcal{H} \,|\, \ell' \rangle \, \langle \ell' \,|\, -\omega\, \delta_{\nu\rho} + \partial_\nu\, \partial_\rho \mathcal{H} \,|\, \ell'' \rangle \, \langle \ell'' \,|\, \partial_\sigma \mathcal{H} \,|\, \ell \rangle}{(e_\ell - e_{\ell'})(e_\ell - e_{\ell''})} \\
& + \sum_{\substack{\ell', \ell'', \ell''' \\ (\neq \ell)}} \frac{\langle \ell \,|\, \partial_\mu \mathcal{H} \,|\, \ell' \rangle \, \langle \ell' \,|\, \partial_\nu \mathcal{H} \,|\, \ell'' \rangle \, \langle \ell'' \,|\, \partial_\rho \mathcal{H} \,|\, \ell''' \rangle \, \langle \ell''' \,|\, \partial_\sigma \mathcal{H} \,|\, \ell \rangle}{(e_\ell - e_{\ell'})(e_\ell - e_{\ell''})(e_\ell - e_{\ell'''})} \,. \qquad \text{(B4)}
\end{aligned}
$$

APPENDIX C

Projectors and derivatives.

We show in this Appendix the following useful result :

$$
\text{For } \ell \neq \ell' , \qquad \frac{\langle \ell \,|\, \partial_\mu \mathcal{H} \,|\, \ell' \rangle}{e_\ell - e_{\ell'}} = \langle \ell \,|\, \partial_\mu P_\ell \,|\, \ell' \rangle \quad \text{holds} . \qquad \text{(C1)}
$$

Using similar ideas, one can derive the Feynmann-Hellman theorem :

$$
\langle \ell \,|\, \partial_\mu \mathcal{H} \,|\, \ell \rangle = \langle \ell \,|\, \ell \rangle \,.\, \partial_\mu e_\ell \,.
$$

To prove (C1), we take the derivative ∂_μ of $\mathcal{H}(\mathbf{k}) = \sum_{\ell''} e_{\ell''}(\mathbf{k})\, P_{\ell''}(\mathbf{k})$, where $P_\ell(\mathbf{k}) \equiv |\ell\rangle_{\mathbf{k}}\, {}_{\mathbf{k}}\langle \ell|$. This leads to :

$$
\partial_\mu \mathcal{H}(\mathbf{k}) = \sum_{\ell''} \partial_\mu e_{\ell''}(\mathbf{k}) \cdot P_{\ell''}(\mathbf{k}) + \sum_{\ell''} e_{\ell''}(\mathbf{k}) \cdot \partial_\mu P_{\ell''}(\mathbf{k}) , \qquad \text{(C2)}
$$

The first term in (C2) is a diagonal matrix, so for $\ell \neq \ell'$:

$$
{}_{\mathbf{k}}\langle \ell \,|\, \partial_\mu \mathcal{H}(\mathbf{k}) \,|\, \ell' \rangle_{\mathbf{k}} = \sum_{\ell''} e_{\ell''}(\mathbf{k})\, {}_{\mathbf{k}}\langle \ell \,|\, \partial_\mu P_{\ell''}(\mathbf{k}) \,|\, \ell' \rangle_{\mathbf{k}} . \qquad \text{(C3)}
$$

But, $P_s(\mathbf{k})$ are projectors :

$$
P_s(\mathbf{k})\, P_t(\mathbf{k}) = 0 \quad \text{if} \quad s \neq t \,; \quad 1 \leqslant s, t \leqslant q \,.
$$

Taking the derivative ∂_μ leads to :

$$
\partial_\mu P_s \,.\, P_t + P_s\, \partial_\mu P_t = 0 , \quad s \neq t \qquad \text{(C4)}
$$

and for $s = t$, $P_s^2 = P_s$ gives : $\partial_\mu P_s \,.\, (1 - P_s) = P_s \,.\, \partial_\mu P_s$.

Using now the definition of P_ℓ as $P_\ell = |\ell\rangle\langle\ell|$ and $\ell'' \neq \ell$, one deduces :

$$\begin{aligned}\langle \ell | \partial_\mu P_{\ell''} | \ell' \rangle &= \langle \ell | P_\ell \, \partial_\mu P_{\ell''} | \ell' \rangle = - \langle \ell | \partial_\mu P_\ell \, . \, P_{\ell''} | \ell' \rangle \\ &= - \delta_{\ell' \ell''} \langle \ell | \partial_\mu P_\ell | \ell' \rangle \, . \end{aligned} \tag{C5}$$

The desired result is a consequence of (C3) and (C5). More elaborated identities can actually be derived, following the same line of arguments.

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