



HAL
open science

A GAUSSIAN BEAM CONSTRUCTION OF DE HAAS-VAN ALFVEN RESONANCES

Mouez Dimassi, Jean-Claude Guillot, James Ralston

► **To cite this version:**

Mouez Dimassi, Jean-Claude Guillot, James Ralston. A GAUSSIAN BEAM CONSTRUCTION OF DE HAAS-VAN ALFVEN RESONANCES. 2024. hal-04716680v1

HAL Id: hal-04716680

<https://hal.science/hal-04716680v1>

Preprint submitted on 1 Oct 2024 (v1), last revised 26 Nov 2024 (v2)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

A GAUSSIAN BEAM CONSTRUCTION OF DE HAAS-VAN ALFVEN RESONANCES

MOUEZ DIMASSI, JEAN-CLAUDE GUILLOT AND JAMES RALSTON

ABSTRACT. In this article we consider a Bloch electron in a crystal lattice subject to slowly varying external magnetic fields. We offer an explanation of de Haas-van Alfvén oscillations in terms of energy levels of approximate eigenfunctions for the magnetic Schrödinger operator by using a gaussian beam construction for a small enough magnetic field.

1. INTRODUCTION

The quantum dynamics of a Bloch electron in a crystal subject to external constant magnetic field $\nabla \times A$ is governed by the Schrödinger equation

$$(1) \quad (P - E_0)u := \left[\frac{\hbar^2}{2m} (D_x + \mu A(x))^2 + eV(x) - E_0 \right] u = 0, \quad D_x = \frac{1}{i} \partial_x,$$

where V is a smooth, real-valued potential, periodic with respect to a lattice $\Gamma = \bigoplus_{i=1}^3 \mathbb{Z}a_i$ in \mathbb{R}^3 . Here (a_1, a_2, a_3) is a basis of \mathbb{R}^3 , m and e are the mass and charge of the electron, and $\mu\hbar = e$. The magnetic potential $A(x) = (0, \epsilon x_1, 0)$ corresponding to the constant magnetic field $\nabla \times A = (0, 0, \epsilon)$. In this paper we will treat the magnetic field strength ϵ as a small parameter and use the scaled variable $y = \epsilon x$ and the potential $A(y) = (0, y_1, 0)$.

In the semi-classical dynamics of Bloch electrons under slowly varying electric and magnetic fields, recent advances have been made (see [?, ?, ?, ?] and the references given there). Since the work of Peierls [?] and Slater [?], it is well known that, if ϵ is sufficiently small, the wave packets are propagating along the trajectories from the semi-classical Hamiltonian $H(y, p) = E(p + \mu A(y))$, $y = \epsilon x$. Here $E(k)$ is one of the band functions describing the Floquet spectrum of the unperturbed Hamiltonian $-\frac{\hbar^2}{2m} \Delta + eV(x)$. In order ϵ , the semi-classical quantization condition for magnetic levels (well-known Onsager relation), contains two phases : One is the Berry's phase, and the other is known as the Wilkinson-Rammal phase (see [?, ?]).

The orbit of the full classical Hamiltonian $H(y, p)$ is helical and cannot be quantized. Its projection on the pseudo-momentum coordinate $k = p + \mu A(y)$ lies in the intersection of the Fermi surface $\{E(k) = E_0\}$ with the plane where k_3 is constant. Under the assumption that this intersection is a simple closed curve, the electron's motion that is perpendicular to the

2000 *Mathematics Subject Classification.* 81Q10 (35P20 47A55 47N50 81Q15).

Key words and phrases. Schrödinger operator, de Haas-van Alfvén oscillations, gaussian beam construction, magnetic field, generalized Onsager relation.

magnetic field is quantized. In order to examine the generalized Onsager relation, we will employ the reduced Peierls classical Hamiltonian, $\hat{H}(y_1, y_2, p_1, p_2) := E(p_1, p_2 + \mu y_1, k_3)$, where k_3 is constant and the variable y_3 is deleted (for more information, consult sections 2-3).

In this work, we use the gaussian beam (GB) to construct for ϵ small enough asymptotic solutions of (??) concentrated in a tube of radius $\epsilon^{1/2}$ around the curve $\Pi_{\hat{y}}\hat{\gamma}$ which is traced by $\hat{y}(s) = (y_1(s), y_2(s))$. Here, $\hat{\gamma} := \{(\hat{y}(s), \hat{p}(s)), s \in [0, T]\}$ is a periodic trajectory for the reduced Hamiltonian $\hat{H}(\hat{y}, \hat{p}) = E(p_1, p_2 + \mu y_1, k_3)$, (see Proposition ?? and Theorem ??).

In section 4, we use these approximate asymptotic solutions to study the generalized semiclassical quantization condition for cyclotron orbits. Due to the wave function being single-valued along a closed orbit, the quantization condition including the Berry, Wilkinson-Rammal (WR), and Maslov phases is established in Theorem ?. It should be noted that the Berry phase and WR phase both involve cell-periodic Bloch wave functions and cannot be derived from the zero-field energy spectrum alone. The geometry of the Bloch states has a crucial impact on the phase of magnetic oscillations.

When $\hat{\gamma}$ is a stable periodic orbit for the bicharacteristic flow, GB is well-understood for a large class of partial differential equations (see [?, ?, ?]). In our case, the curve $\hat{\gamma}$ is unstable (i.e., all the eigenvalues of the linearized Poincare are real). The construction of quasi-modes in [?, ?] and elsewhere does not allow this. To remove this difficulty, we will examine and adapt more closely Ralston's approach to our case.

2. PRELIMINARIES

Equations of motion in Physical and Pseudo-momentum spaces. Let $E_n(k)$ be one of the band functions describing the Floquet spectrum of the unperturbed Hamiltonian:

$$H_0(k) = \frac{\hbar^2}{2m}(D_x + k)^2 + eV(x) : L^2(\mathbb{T}) \rightarrow L^2(\mathbb{T}).$$

Let $\Phi_n(\cdot, k) = e^{-ix \cdot k} \Psi_n(x, k)$ be the corresponding normalized eigenfunction,

$$(2) \quad \left[H_0(k) - E_n(k) \right] \Phi_n(x, k) = 0, \quad \int_{\mathbb{T}} |\Phi_n(x, k)|^2 dx = 1,$$

where $\Psi_n(\cdot, k)$ is the Bloch function associated to $E_n(k)$:

$$\Psi_n(x + \gamma, k) = e^{ik \cdot \gamma} \Psi_n(x, k), \quad \forall \gamma \in \Gamma.$$

Since $e^{-ix \cdot \gamma^*} H_0(k) e^{ix \cdot \gamma^*} = H_0(k + \gamma^*)$, it follows that that

$$E_n(k + \gamma^*) = E_n(k), \quad \text{for all } \gamma^* \in \Gamma^*,$$

where Γ^* is the reciprocal lattice. Standard perturbation theory shows that the function $E_n(k)$ is continuous for $k \in \mathbb{R}^3$ and real analytic in a neighborhood of any k such that

$E_n(k)$ is a simple eigenvalue, i.e.,

$$E_{n-1}(k) < E_n(k) < E_{n+1}(k).$$

For $E_0 \in E_n(\mathbb{T}^*)$, we put $\mathcal{F}(E_0) = \{k \in \mathbb{T}^* : E_n(k) = E_0\}$ ¹. We assume that for every $k = (k_1, k_2, k_3) \in \mathcal{F}(E_0)$ with k_3 in an open interval, $E_n(k)$ is a simple eigenvalue of $H_0(k)$. Therefore, $k \mapsto E_n(k)$ is analytic in a neighborhood of $\mathcal{F}(E_0)$, and we can choose $k \mapsto \Psi_{n_0}(\cdot, k)$ to be a real-analytic function near $\mathcal{F}(E_0)$. Since we will use only one band, we will suppress the index n in $E_n(k)$, $\Phi_n(\cdot, k)$ and $\Psi_n(\cdot, k)$.

In classical discussions ([?]) the de Haas-van Alfvén effect is associated with the curves in pseudo-momentum space obtained as intersections of planes perpendicular to the (constant) magnetic field with the Fermi surface. Here we use the curves in (y_1, y_2, p_1, p_2) corresponding to electron paths. These curves are determined by the Peierls Hamiltonian $H(y, p) = E(p + \mu A)$. However, they are obtained from the pseudo-momentum space curves above by substituting $k_1 = p_1, k_2 = p_2 + \mu y_1$ and $k_3 = p_3$, and setting $y_2 = -\frac{p_2}{\mu}$ plus a constant (our constructions will be independent of y_3). To verify this we compute as follows. Let $(y(s), p(s))$ be a trajectory for the Peierls hamiltonian generated by $H(y, p)$:

$$(3) \quad \dot{y}(s) = \frac{\partial H}{\partial p} = \frac{\partial E}{\partial k}(p(s) + \mu A(y(s))),$$

$$(4) \quad \dot{p}(s) = -\frac{\partial H}{\partial y} = -\mu(\dot{y}_2(s), 0, 0).$$

In the pseudo-momentum coordinate $k(s) := p(s) + \mu A(y(s))$ one has

$$E(k(s)) = E(k_1(s), k_2(s), k_3) = E(k(0)) = E_0,$$

and

$$(5) \quad \dot{y}(s) = \frac{\partial E}{\partial k}(k(s)), \quad \dot{k}(s) = \mu(-\dot{y}_2(s), \dot{y}_1(s), 0).$$

Let $z_1 = p_2 + \mu y_1$. Since $\dot{p}_2 = 0$, we have

$$\dot{z}_1 = \mu \frac{\partial E}{\partial k_1}(p_1, z_1, p_3) \text{ and } \dot{p}_1 = -\mu \frac{\partial E}{\partial k_2}(p_1, z_1, p_3).$$

Hence, since $\dot{p}_3 = 0$, $(z_1(s), p_1(s))$ moves along a level curve for $E(p_1, z_1, k_3)$. We also have

$$(6) \quad \dot{y}_2 = \partial_{p_2} E(p_1, p_2 + \mu y_1, p_3) = -\dot{p}_1/\mu.$$

Thus there are two families of trajectories here. First there the level curves

$$\gamma = \gamma(k_3, E_0) = \{(k_1, k_2) : E(k_1, k_2, k_3) = E_0\}.$$

Second there are the trajectories (with y_3 deleted) for the Peierls Hamiltonian

$$(7) \quad \hat{\gamma} = \hat{\gamma}(k_3, E_0, c) = \{(y_1, y_2, p_1, p_2) : E(p_1, p_2 + \mu y_1, k_3) = E_0, y_2 = -p_1/\mu + c\}.$$

¹When E_0 equals the Fermi energy E_F , $\mathcal{F}(E_0)$ is part of the Fermi surface defined by $\mathcal{F}_F := \{k \in \mathbb{T}^*; E_F \in \sigma(H_0(k))\}$ (see [?]). Here $\sigma(H_0(k))$ denotes the spectrum of the operator $H_0(k)$.

Note that $\gamma(k_3, E_0)$ will become $\hat{\gamma}(k_3, E_0, c)$ when one substitutes $k_1 = p_1$ and $k_2 = p_2 + \mu y_1$ and sets $y_2 = -p_1/\mu + c$. $\hat{\gamma}$ will be used in the sections Generalized Onsager Relation.

Throughout this paper we assume that :

$$(H1) \quad \left(\frac{\partial E}{\partial k_1}, \frac{\partial E}{\partial k_2} \right) \neq (0, 0) \text{ on } \gamma(k_3, E_0),$$

and

$$(H2) \quad \gamma(k_3, E_0) \text{ is a simple closed curve.}$$

Assumptions (H1) and (H2) insure that $\{(k_1, k_2) : E(k_1, k_2, t_3) = E\}$ are simple and closed for $|E - E_0|$ and $|t_3 - k_3|$ small enough and that it depends smoothly on (t_3, E) .

We let $S(k_3)$ denote the area in k -space enclosed by $\gamma(k_3, E_0)$. $\gamma(k_3, E_0)$ is the projection of a helical orbit $\hat{\Gamma}(k_3)$ of the full hamiltonian in (??), (??).

3. GAUSSIAN BEAM CONSTRUCTION

3.1. Two scale expansions method, eikonal and transports equations. In what follows, \hat{y} (resp. \hat{x}, \hat{k}) denotes (y_1, y_2) (resp. $(x_1, x_2), \hat{k} = (k_1, k_2)$). With the change of variable $\hat{y} = \epsilon \hat{x}$, the operator P is unitarily equivalent to

$$\tilde{P} = \frac{\hbar^2}{2m} \left[(\epsilon D_{\hat{y}} + \mu A(\hat{y}))^2 + D_{x_3}^2 \right] + eV\left(\frac{\hat{y}}{\epsilon}, x_3\right).$$

Here we are looking for a solution of the equation

$$(8) \quad (\tilde{P} - E_0)u(\hat{y}, x_3, \epsilon) \equiv 0.$$

of the form

$$u(\hat{y}, x_3, \epsilon) = e^{i(\phi(\hat{y})/\epsilon + x_3 k_3)} m\left(\frac{\hat{y}}{\epsilon}, x_3, \hat{y}; \epsilon\right).$$

In order to accomplish this we use, as in [?, ?, ?], the two-scale expansion method in which the coordinate \hat{x} and the slowly varying space variable $\hat{y} = \epsilon \hat{x}$ are regarded as independent variables. Thus, we consider the following equation in the independent variables \hat{x} and \hat{y} :

$$(9) \quad (\mathbb{P} - E_0)v = 0,$$

with

$$(10) \quad \mathbb{P} = \frac{\hbar^2}{2m} \left[(\epsilon D_{\hat{y}} + D_{\hat{x}} + \mu A(\hat{y}))^2 + (D_{x_3} + k_3)^2 \right] + eV(\hat{x}, x_3)$$

Note that, if $v(\hat{x}, x_3, \hat{y}, \epsilon)$ is a solution of (9), then $u = e^{ix_3 k_3} v\left(\frac{\hat{x}}{\epsilon}, x_3, \hat{y}, \epsilon\right)$ is a solution of (8). In the variable $x = (\hat{x}, x_3)$, $v(x, \hat{y}, \epsilon)$ is required to be periodic.

We look for approximate solution to (9), which have the form :

$$(11) \quad v(\hat{x}, x_3, \hat{y}, \epsilon) = e^{i\phi(\hat{y})/\epsilon} \left[m_0(\hat{x}, x_3, \hat{y}) + \epsilon m_1(\hat{x}, x_3, \hat{y}) + \dots + \epsilon^N m_N(\hat{x}, x_3, \hat{y}) \right].$$

Now substituting (??) into (??) and collecting terms which are the same order in ϵ , we get

$$(12) \quad (\mathbb{P} - E_0)v = e^{i\phi(\hat{y})/\epsilon} \left[c_0(\hat{x}, x_3, \hat{y}) + \epsilon c_1(\hat{x}, x_3, \hat{y}) + \cdots + \epsilon^{N+2} c_{N+2}(\hat{x}, x_3, \hat{y}) \right]$$

where

$$(13) \quad c_0(\hat{x}, x_3, \hat{y}) = [H_0(K(\hat{y})) - E_0] m_0,$$

$$(14) \quad c_1(\hat{x}, x_3, \hat{y}) = [H_0(K(\hat{y})) - E_0] m_1 - \frac{\hbar^2}{2m} \mathbb{K} m_0,$$

and for $j = 2, 3, \dots, N + 2$

$$c_j(\hat{x}, x_3, \hat{y}) = [H_0(K(\hat{y})) - E_0] m_j - \frac{\hbar^2}{2m} \left(\mathbb{K} m_{j-1} + \Delta_{\hat{y}} m_{j-2} \right).$$

Here

$$\mathbb{K} = i \left[\frac{\partial H_0}{\partial \hat{k}}(K(\hat{y})) \cdot \frac{\partial}{\partial \hat{y}} + \Delta_{\hat{y}} \phi \right]$$

and

$$K(\hat{y}) = \left(\frac{\partial \phi}{\partial \hat{y}}(\hat{y}) + \mu A(\hat{y}), k_3 \right).$$

When ϕ is real-valued, (??) is the standard ansatz of the WKB-method. In this case, to solve the equation (??), one requires that $c_j = 0, j = 0, 1, 2, \dots$:

$$(E) \quad c_0 = [H_0(K(\hat{y})) - E_0] m_0 = 0, \quad (\text{eikonal equation})$$

$$(T_1) \quad c_1 = [H_0(K(\hat{y})) - E_0] m_1 - \frac{\hbar^2}{2m} \mathbb{K} m_0 = 0, \quad (\text{transport equation } T_1)$$

$$(T_j) \quad c_j(\hat{x}, x_3, \hat{y}) = 0, \quad (\text{transport equation } T_j).$$

3.2. Construction of the phase function by the Gaussian beam method. According to (??), equation tells us that for all \hat{y} , $m_0(\hat{x}, x_3, \hat{y})$ is an eigenfunction of $H_0(K(\hat{y}))$ with eigenvalue E_0 . Therefore, we can fulfill (??) by choosing

$$(E_\phi) \quad E \left(\frac{\partial \phi}{\partial \hat{y}}(\hat{y}) + \mu A(\hat{y}), k_3 \right) = E_0,$$

$$m_0(\hat{x}, x_3, \hat{y}) = f_0(\hat{y}) \Phi(x, K(\hat{y})).$$

The phase ϕ is derived from the classical hamiltonian

$$\widehat{H}(\hat{y}, \hat{p}) := \widehat{H}(y_1, y_2, p_1, p_2) = E(p_1, p_2 + \mu y_1, k_3).$$

By definition (see (??)), $\hat{\gamma}$ is a periodic orbit for the Hamiltonian system

$$(15-0) \quad \dot{\hat{y}} = \widehat{H}_p, \quad \dot{\hat{p}} = -\widehat{H}_y.$$

Along $\hat{\gamma}$, ϕ satisfies $(p_1(s), p_2(s)) = \phi_y(y(s))$ with

$$(15-1) \quad E(k(s)) = E_0, \quad k(s) = (p_1(s), p_2(s) + \mu y_1(s), k_3) = (\phi_{\hat{y}}(\hat{y}(s)) + \mu A(\hat{y}(s)), k_3).$$

The nonlinearity of the Hamilton-Jacobi equation (??) generally leads to finite time singularity formation in phase ϕ "caustic problem", and the transport equations then become undefined. The caustic problem has been addressed in many works, starting with Keller, Maslov, and Hörmander, using the classical Fourier integral operator (FIO) approach [?]. As indicated in the introduction, instead of OIF we are going to use "Gaussian Beams" as in [?, ?, ?]. This means that we are not going to attempt to solve (??) exactly, we only need to build asymptotic solutions concentrated on a single ray $\hat{\gamma}$. The Gaussian profile is achieved by allowing the phase to be complex away from the ray so that the solution decays exponentially away from $\hat{\gamma}$.

More precisely, fix a periodic trajectory $\hat{\gamma} = \{(\hat{y}(s), \hat{p}(s)); s \in [0, T]\}$ of the classical hamiltonian \hat{H} with initial date $(\hat{y}(0), \hat{p}(0))$ satisfying $\hat{H}(\hat{y}(0), \hat{p}(0)) = E_0$, and let $\Pi_{\hat{y}}\hat{\gamma}$ denote the projection of $\hat{\gamma}$ on the \hat{y} -space. We are going to prove

Proposition 1. *Assume (??) and (??). There exists a smooth function ϕ such that*

- i) $\frac{\partial \phi}{\partial \hat{y}}(\hat{y}(s)) = \hat{p}(s)$.
- ii) *In a small neighborhood Ω of $\Pi_{\hat{y}}\hat{\gamma}$*

$$(15) \quad G(y) := E\left(\frac{\partial \phi}{\partial \hat{y}}(\hat{y}) + \mu A(\hat{y}), k_3\right) - E_0 = \mathcal{O}_N\left(d(\hat{y}, \Pi_{\hat{y}}\hat{\gamma})^3\right),$$

- iii) $\Im \phi \geq Cd(\hat{y}, \Pi_{\hat{y}}\hat{\gamma})^2$,

where $d(\hat{y}, \Pi_{\hat{y}}\hat{\gamma})$ is the distance from \hat{y} to $\Pi_{\hat{y}}\hat{\gamma}$.

Proof. The proof is adapted from [?]. For this reason we omit some details. Here, the main difficulty in carrying out the construction in [?] is that all orbits for \hat{H} near $\hat{\gamma}$ are periodic, hence the algebraic eigenvalues of the linearized Poincare map \mathcal{P} are all 1. This is not allowed in the construction of quasi-modes in [?] and elsewhere.

Recall that k_3 is fixed, and the classical hamiltonian $\hat{H}(y_1, y_2, p_1, p_2) = E(p_1, p_2 + \mu y_1, k_3)$ is independent on y_3 . By abuse of notation, we write $y, y(s), p, H$ instead of $\hat{y} = (y_1, y_2)$, $\hat{y}(s) = (y_1(s), y_2(s))$, $\hat{p} = (p_1, p_2)$, and \hat{H} .

Requiring that $G(y) = H(y, \frac{\partial \phi}{\partial y}(y)) - E_0$ vanishes to zero, first and second order on $\hat{\gamma}$, we get :

1. $\frac{\partial \phi}{\partial y}(y(s)) = p(s)$,
2. $\frac{\partial G}{\partial y_j} = \frac{\partial H}{\partial y_j} + \sum_{l=1,2} \frac{\partial H}{\partial p_l} \frac{\partial^2 \phi}{\partial y_j \partial y_l} = 0$, for $j = 1, 2$,
3. $\frac{\partial^2 G}{\partial y_i \partial y_j} = \frac{\partial^2 H}{\partial y_i \partial y_j} + \sum_{l=1,2} \left(\frac{\partial^2 \phi}{\partial y_i \partial y_l} \frac{\partial^2 H}{\partial p_l \partial y_j} + \frac{\partial^2 H}{\partial y_i \partial p_l} \frac{\partial^2 \phi}{\partial y_l \partial y_j} + \frac{\partial H}{\partial p_l} \frac{\partial^3 \phi}{\partial y_l \partial y_i \partial y_j} \right) = 0$ for $i, j = 1, 2$,
where the equalities are evaluated along $\hat{\gamma}$.

It's worth noting that 1. is a consequence of the uniqueness of the solution of (??) with initial condition. While 2. is only the compatibility condition $\dot{p}(s) = \frac{d}{ds}\left(\frac{\partial \phi}{\partial y}(y(s))\right)$. Let us investigate the third condition.

Introducing the matrix

$$\begin{aligned} (M(s))_{ij} &= \frac{\partial^2 \phi}{\partial y_i \partial y_j}(y(s)), & (A(s))_{ij} &= \frac{\partial^2 H}{\partial y_i \partial y_j}(y(s), p(s)), \\ (B(s))_{ij} &= \frac{\partial^2 H}{\partial p_i \partial y_j}(y(s), p(s)), & (C(s))_{ij} &= \frac{\partial^2 H}{\partial p_i \partial p_j}(y(s), p(s)), \end{aligned}$$

and using (??), one can rewrite the condition 3) as the non-linear Ricatti matrix equation

$$(RE) \quad \frac{dM}{ds} + MCM + MB + B^T M + A = 0.$$

Thus in order to prove Proposition 1, we need to construct a phase ϕ such the the matrix $M(s)$ satisfies (??) for all s with

- $M(s)^T = M(s)$,
- $M(s + T) = M(s)$,
- $M(s)\dot{y}(s) = \dot{p}(s)$,
- $\Im M(s)$ is positive definite on the orthogonal complement of $\dot{y}(s)$,

Some well known facts about the non-linear Ricatti equation (??) are recalled in an appendix.

Next, let us introduce the linearized equation about $\hat{\gamma}$

$$(16) \quad \begin{cases} \dot{\delta y} = C(s)\delta p + B(s)\delta y \\ \dot{\delta p} = -B^T(s)\delta p - A(s)\delta y, \end{cases}$$

and the linearized Poincaré map \mathcal{P} taking the data of solutions to (??) at $s = 0$ to their data at $s = T$, (i.e., $\mathcal{P} : (\delta y(0), \delta p(0)) \rightarrow (\delta y(T), \delta p(T))$).

To apply the arguments from [?], we need two vector solutions of (??), $v_1(s)$ and $v_2(s)$, where $v_1(s)$ is the tangent to $\hat{\gamma}$, i.e. $v_1 = (\dot{y}_1, \dot{y}_2, \dot{p}_1, \dot{p}_2(= 0))$ which will satisfy (??) because it is the derivative of the flow of H with respect to s .

Since we have assumed that $v_1(s)$ is never zero, $v_2(s)$ must satisfy three conditions. Letting $\sigma((y, \eta), (w, \zeta)) = y \cdot \zeta - w \cdot \eta$ be the symplectic two form, we need :

- i) $\sigma(v_2(s), \underline{v_1(s)}) = 0$ for all s .
- ii) $\sigma(v_2(s), v_2(s)) = ic$ with $c > 0$ for all s .
- iii) The complex span of $v_1(s)$ and $v_2(s)$, $S(s)$ should be periodic, i.e. $S(0) = S(T)$.

Since σ is constant on pairs of solutions to (??) (see (??)), the equalities i) and ii) will hold for all s , if they hold for $s = 0$. Condition iii) makes this construction possible in our special case. The fact that all orbits near $\hat{\gamma} = \hat{\gamma}(E_0, k_3)$ are periodic means that for any solution $v(s)$ of (??), \mathcal{P} maps $v(0)$ to $v(0) + av_1(0)$ for some a . To see this choose curves $w_1(s)$ and $w_2(s)$ in (y, p) -space such that $w_1(0) = w_2(0)$ is on γ , and $\dot{w}_1(0) + i\dot{w}_2(0) = v_2(0)$. Recalling that the level surface $\{(y, p), \hat{H}(y, p) = E\}$ is 3-dimensional for $|E - E_0|$ small enough, due to the assumption (??). Since all orbits are periodic, $w_1(s)$ and $w_2(s)$

are on periodic orbits, $w_1(t, s)$ and $w_2(t, s)$ respectively. Note that $w_1(t, 0)$ and $w_2(t, 0)$ parametrize γ and hence there are functions $T_1(s)$ and $T_2(s)$ such that

$$(16-0) \quad w_1(T_1(s), s) = w_1(0, s) \text{ and } w_2(T_2(s), s) = w_2(0, s).$$

Evaluating the derivatives of the equations in (??) with respect to s at $s = 0$, we have (since $T_j(0) = T$)

$$\partial_s w_j(0, 0) = \partial_s w_j(T, 0) + \partial_s T_j(0) \partial_t w_j(T, 0), \quad j = 1, 2,$$

which yields $v_2(0) = v_2(T) + (\partial_s T_1(0) + i \partial_s T_2(0)) v_1(T)$.

Therefore, $S(T) = S(0)$ for any choice of $v_2(s)$, and we have plenty of freedom to choose $v_2(0)$ so that i) and ii) hold. For instance, we could choose $(y(0), p(0))$ so that $\dot{y}_1(0) \neq 0$, and let $v_2(s) = (\delta y_1^2(s), \delta y_2^2(s), \delta p_1^2(s), \delta p_2^2(s))$ with $v_2(0) = (0, i \dot{y}_1(0), -\dot{y}_2(0), \dot{y}_1(0))$. Let us introduce the 2×2 matrices

$$Y(s) := (Y^1(s), Y^2(s)) = \begin{pmatrix} \dot{y}_1(s) & \delta y_1^2(s) \\ \dot{y}_2(s) & \delta y_2^2(s) \end{pmatrix}, \quad N(s) := (N^1(s), N^2(s)) = \begin{pmatrix} \dot{p}_1(s) & \delta p_1^2(s) \\ \dot{p}_2(s) & \delta p_2^2(s) \end{pmatrix}.$$

Since we assumed that $(\dot{y}_1(s), \dot{y}_2(s))$ never vanishes (see (??) and (??)), we conclude from Proposition ?? that $Y(s)$ is invertible for all s , hence that $M(s) = N(s)Y(s)^{-1}$ is well defined for all s , and finally that $M(s)$ is a global solution of (??).

Now, the desired properties of the matrix $M(s)$ are derived from Proposition ?? and the fact that $S(0) = S(T)$. This completes the proof of Proposition ?. \square

3.3. Construction of the Amplitude. Constructing the principal term m_0 is all we need to do for the applications. We offer suggestions on how to create the other terms in a remark.

In the following, we assume that ϕ has been chosen so that Proposition ?? holds, and we let $m_0 = f_0(y)\Phi(x, K(y))$. Therefore

$$(17) \quad c_0 = f_0(y)G(y)\Phi(x, K(y)).$$

We want to choose m_0, m_1, \dots , so that the functions $y \rightarrow c_j(x, y)$ vanish on $\hat{\gamma}$ to given order uniformly on $x \in \mathbb{T}$.

First, let us deal with c_0 and c_1 . For simplicity of notation, we write E, H_0 and Φ instead of $E(K(\hat{y})), H_0(K(\hat{y}))$ and $\Phi(x, K(\hat{y}))$ respectively.

Since $x \rightarrow m_1(x, \cdot)$ is required to be Γ -periodic, it is natural to write

$$(18) \quad m_1(x, y) = f_1(y)\Phi(x, K(y)) + m_1^\perp(x, y),$$

where

$$\langle \Phi(\cdot, K(y)), m_1^\perp(\cdot, y) \rangle = 0.$$

Substituting the above equalities into (??) and using (??) we obtain

$$(19) \quad c_1 = f_1(y)G(y)\Phi(x, K(y)) - \frac{\hbar^2}{2m} \mathbb{K}m_0 + [H_0(K(y)) - E_0] m_1^\perp.$$

By the Fredholm alternative, the equation, $c_1 = 0$, is solvable for m_1 if and only if

$$f_1(y)G(y)\Phi(\cdot, K(y)) - \frac{\hbar^2}{2m}\mathbb{K}m_0 \perp \ker [H_0 - E_0] \text{ in } L^2(\mathbb{T}),$$

for all y , i.e.,

$$(20) \quad iL(y) := \left\langle \mathbb{K}(f_0\Phi), \Phi \right\rangle_{L^2(\mathbb{T})} - \frac{2m}{\hbar^2}f_1(y)G(y) = 0.$$

In view of the definition of \mathbb{K} , we have

$$(21) \quad L(y) = \frac{\partial f_0}{\partial y} \cdot \left\langle \frac{\partial H_0}{\partial k} \Phi, \Phi \right\rangle + b(y)f_0(y) - \frac{2m}{i\hbar^2}f_1(y)G(y),$$

where

$$(22) \quad b(y) := \left\langle \frac{\partial H_0}{\partial k} \cdot \frac{\partial \Phi}{\partial y}, \Phi \right\rangle + \Delta_y \phi.$$

We conclude from (??) that

$$(23) \quad \frac{\partial E}{\partial k} \Phi + (E - H_0) \frac{\partial \Phi}{\partial k} = \frac{\partial H_0}{\partial k} \Phi,$$

hence that

$$\frac{\partial E}{\partial k} = \left\langle \frac{\partial H_0}{\partial k} \phi, \phi \right\rangle.$$

Differentiating the above equality with respect to y , and noting that $\frac{\partial H_0}{\partial k}$ is self-adjoint, we get

$$(24) \quad \frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k} = \left\langle \frac{\partial H_0}{\partial k} \frac{\partial \phi}{\partial y}, \phi \right\rangle + \left\langle \frac{\partial H_0}{\partial k} \phi, \frac{\partial \phi}{\partial y} \right\rangle + 2\Delta_y \phi = 2\Re b(y).$$

Inserting (??) in (??) we obtain

$$(25) \quad \Im b = \Im \left\{ \frac{\partial E}{\partial k} \cdot \left\langle \frac{\partial \Phi}{\partial y}, \Phi \right\rangle \right\} + \Im \left\{ \left\langle \frac{\partial \Phi}{\partial y}, (E - H_0) \frac{\partial \Phi}{\partial k} \right\rangle \right\}.$$

Using the fact that $\left\langle \frac{\partial \Phi}{\partial k_j}, (E - H_0) \frac{\partial \Phi}{\partial k_j} \right\rangle$ is real, as well as the fact that $\frac{\partial K_2}{\partial y_1} - \frac{\partial K_1}{\partial y_2} = \mu$, we deduce that

$$\Im \left\{ \left\langle \frac{\partial \Phi}{\partial y}, (E - H_0) \frac{\partial \Phi}{\partial k} \right\rangle \right\} = \mu \Im \left\langle (H_0 - E) \frac{\partial \Phi}{\partial k_1}, \frac{\partial \Phi}{\partial k_2} \right\rangle.$$

On the other hand, the normalization of Φ ensures that $\frac{1}{i} \left\langle \frac{\partial \Phi}{\partial y}, \Phi \right\rangle$ is real. This, together with (??), (??) and (??) yields

$$(26) \quad L(y) = \frac{\partial E}{\partial k} \cdot \frac{\partial f_0}{\partial y} + \mathcal{A}(y)f_0(y) - \frac{2m}{i\hbar^2}f_1(y)G(y),$$

where

$$\mathcal{A}(y) := \frac{1}{2} \frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k} + i \left(\mu \Im \left\langle \frac{\partial \Phi}{\partial k_2}, (E - H_0) \frac{\partial \Phi}{\partial k_1} \right\rangle + \frac{1}{i} \frac{\partial E}{\partial k} \cdot \left\langle \frac{\partial \Phi}{\partial y}, \Phi \right\rangle \right).$$

It is worth recalling that we want to choose f_0 and f_1 such that the right hand side of (??) vanishes on $\hat{\gamma}$ to given order. For any multi-index α of length l the equations $\partial_y^\alpha L(y) = 0$

along $\hat{\gamma}$ gives rise to linear ordinary differential equation for $\partial_y^\alpha f_0$ with inhomogeneous terms depending on the derivatives of f_0 and f_1 of order up to $l-1$ and $l-3$ respectively :

$$(27) \quad \frac{\partial E}{\partial k} \cdot \frac{\partial}{\partial y} (\partial_y^\alpha f_0) + \mathcal{A}(y) \partial_y^\alpha f_0(y) + C(f_0, \dots, \partial_y^\beta f_0, f_1, \dots, \partial_y^{\beta'} f_1) = 0,$$

with $|\beta'| \leq l-3$, $|\beta| \leq l-1$ and C is independent on f_1 for $l < 3$ and $C = 0$ for $\alpha = 0$. Here we have used (??).

Since $\dot{y}(s) = \frac{\partial E}{\partial k}$, it follows from (??) and the definition of $A(y)$ that :

$$(28) \quad \frac{d}{ds} \left[(\partial_y^\alpha f_0)(y(s)) \right] + \frac{1}{2} \left(\partial_y \cdot \partial_k E(\phi_y + \mu A(y), k_3) \right)_{|y(s)} (\partial_y^\alpha f_0)(y(s)) + i \left(\dot{\theta}_b + \dot{\theta}_{rw} \right) (\partial_y^\alpha f_0)(y(s)) \\ + C(f_0, \partial_y f_0, \dots, \partial_y^\beta f_0, f_1, \dots, \partial_y^{\beta'} f_1)_{|y=y(s)} = 0,$$

where, the phase θ_b is known as the Berry phase and θ_{rw} is the Wilkinson-Rammal phase :

$$(29) \quad \dot{\theta}_b = i \left\langle \Phi(\cdot, k(s)), \dot{\Phi}(\cdot, k(s)) \right\rangle,$$

and

$$(30) \quad \dot{\theta}_{rw} = \Im \left\langle (H_0(k(s)) - E_0) \frac{\partial \Phi}{\partial k_1}(\cdot, k(s)), \frac{\partial \Phi}{\partial k_2}(\cdot, k(s)) \right\rangle.$$

To solve (??) for the partial derivatives of f_0 on $\hat{\gamma}$ up to order l , we may assume that f_1 vanish to order $l-2$ at all points of $\hat{\gamma}$. Thus, the right hand side of (??) is no longer dependent on f_1 . Since the coefficient C depends on all the partials of f_0 up to order $l-1$, we can solve (??) recursively. By linearity the solution exists for *all* s . Thus, it suffices to prescribe $\partial_y^\alpha f_0(y(0))$ for $|\alpha| = l$, to get the l^{th} order partial derivatives of f_0 on the whole curve $\hat{\gamma}$. Therefore, we may assume that f_0 is chosen so that for given $l \in \mathbb{N}$ the left hand side of (??) vanishes to order l on $\hat{\gamma}$, i.e.,

$$(31) \quad \left\langle \mathbb{K}(f_0 \Phi), \Phi \right\rangle = \mathcal{O} \left(d(y, \Pi_y \hat{\gamma})^{l+1} \right).$$

This completes the construction of m_0 .

Remark 2. To compute the other terms m_1, m_2, \dots , we proceed as follows. Set

$$(32) \quad m_1^\perp = \frac{\hbar^2}{2m} (H_0 - E_0)^{-1} \left(\mathbb{K}m_0 - \langle \mathbb{K}m_0, \Phi \rangle \Phi \right) = \frac{\hbar^2}{2m} (H_0 - E_0)^{-1} \left(\mathbb{K}m_0 \right),$$

where $(H_0 - E_0)^{-1}$ denotes the inverse which maps the orthogonal complement of Φ in $L^2(\mathbb{T})$ into itself. According to (??) we need only to compute f_1 . We recall that f_1 needs to vanish to order $l-2$ at all points of $\hat{\gamma}$, and G satisfies (??). Combining this with (??), (??), (??) and (??) we get

$$(33) \quad c_1 = \mathcal{O} \left(d(y, \Pi_y \hat{\gamma})^{l+1} \right)$$

uniformly on $x \in \mathbb{T}$. Like T_1 , T_2 can be solved for $m_2 = f_2 \Phi + m_2^\perp$ if and only

$$(34) \quad \left\langle \mathbb{K}(f_1 \Phi), \Phi \right\rangle_{L^2(\mathbb{T})} = \frac{2m}{\hbar^2} f_2(y) G(y) - \left\langle \mathbb{K}(m_1^\perp), \Phi \right\rangle_{L^2(\mathbb{T})} - \left\langle \Delta_y(m_0), \Phi \right\rangle_{L^2(\mathbb{T})}.$$

The left side of the above equality is identical to that of (??) with f_1 instead of f_0 . Therefore, as in the proof of (??), equation (??) gives

$$(35) \quad L_1(y) := \frac{\partial E}{\partial k} \cdot \frac{\partial f_1}{\partial y} + \mathcal{A}(y)f_1(y) - \frac{2m}{i\hbar^2}f_2(y)G(y) + \frac{1}{i} \left[\left\langle \mathbb{K}(m_1^\perp), \Phi \right\rangle_{L^2(\mathbb{T})} + \left\langle \Delta_y(m_0), \Phi \right\rangle_{L^2(\mathbb{T})} \right] = 0.$$

Notice that the terms inside $[\dots]$ vanish to order $l-2$ on $\hat{\gamma}$. This follows from the definition of m_0 and m_1^\perp and the fact f_0 vanishes to order l on $\hat{\gamma}$.

Remembering that we want to construct f_1 satisfying (??) with $f_1(y) = \mathcal{O}(d(y, \Pi_y \hat{\gamma})^{l-2})$.

As in the proof of (??) (with $l-2$ instead of l), equation (??) shows that for any multi-index α of length $l-2$ the equality $\partial_y^\alpha L_1(y) = 0$ along $\hat{\gamma}$ yields a linear o.d.f. with an inhomogeneous term, F , involving m_0 and m_1^\perp :

$$(36) \quad \frac{\partial E}{\partial k} \cdot \frac{\partial}{\partial y} (\partial_y^\alpha f_1) + \mathcal{A}(y) \partial_y^\alpha f_1(y) + C_1(f_1, \dots, \partial_y^\beta f_1, f_2, \dots, \partial_y^{\beta'} f_2) = F.$$

We get a linear differential equation for the $|\alpha|$ -order partial derivatives of f_1 on $\hat{\gamma}$ with an inhomogeneous term previously determined. We can now proceed analogously to the proof of f_0 .

Let $\hat{\gamma} = \{(\hat{y}(s), \hat{p}(s)); s \in [0, T]\}$ be the null bicharacteristic of the classical Hamiltonian \hat{H} with initial date $(\hat{y}(0), \hat{p}(0))$ satisfying $\hat{H}(\hat{y}(0), \hat{p}(0)) = E_0$, and let $\Pi_{\hat{y}} \hat{\gamma}$ denote the projection of $\hat{\gamma}$ on the \hat{y} -space. Let ϕ the phase given by Proposition 1. Next, we use the above construction for both m_0 and m_1 with $l = 0$, $f_0(\hat{y}(0)) = 1$ and $f_1(\hat{y}(0)) = 0$. Let $\tilde{\Omega} \subset \mathbb{R}^2$ be a small neighborhood of $\Pi_y \hat{\gamma}$, and let $f \in C_0^\infty(\tilde{\Omega})$ be equal one near $\Pi_y \hat{\gamma}$. Put

$$\tilde{u}(\hat{y}, x_3, \epsilon) = e^{i(\phi(\hat{y})/\epsilon + x_3 k_3)} f(\hat{y}) \left(m_0\left(\frac{\hat{y}}{\epsilon}, x_3, \hat{y}\right) + \epsilon m_1\left(\frac{\hat{y}}{\epsilon}, x_3, \hat{y}\right) \right).$$

A small enough $\tilde{\Omega}$ can be selected to ensure that the function f is well defined on the support of ϕ .

We state our main result of this section as follows :

Theorem 3. *Assume (??) and (??). There exists ϵ_0 small enough such that the preceding construction gives an approximate eigenfunction \tilde{u} satisfying :*

- $|(\tilde{P} - E_0)\tilde{u}(\hat{y}, x_3, \epsilon)| \leq C\epsilon^{3/2}$, $(\hat{y}, x_3) \in \mathbb{R}^3$.
- $x \rightarrow m_j(x, \hat{y})$ is periodic.
-

$$\|(\tilde{P} - E_0)\tilde{u}\|_{L^2(\mathbb{R}_{y_1, y_1}^2)} = \mathcal{O}(\epsilon^{3/2}) \|\tilde{u}\|_{L^2(\mathbb{R}_{y_1, y_1}^2)}.$$

uniformly on $\epsilon \in]0, \epsilon_0[$.

- Along $\hat{\gamma}$, we have

$$(37) \quad \tilde{u}(\hat{y}(t), x_3, \epsilon) = e^{i(c(t)/\epsilon - \theta(t) + x_3 k_3)} \sqrt{\frac{\det(Y(0))}{\det(Y(t))}} \Phi\left(\frac{\hat{y}(t)}{\epsilon}, x_3, K(\hat{y}(t))\right) + \mathcal{O}(\epsilon),$$

where

$$c(t) = \int_0^t \hat{p}(s) d\hat{y}(s), \quad \theta(t) = \int_0^t \dot{\theta}_b + \dot{\theta}_{rw} ds.$$

Remark 4. Our solution in (??) involves the square root of the complex number $\det(Y(s))$, and will be sensitive to the number of times the phase of $\det(Y(s))$ wraps around the origin as s goes from zero to T . If this winding number (or Maslov index) is called N_M , we have by Cauchy's argument principle :

$$N_M = \frac{1}{2\pi i} \int_0^T \frac{\partial_s \det(Y(s))}{\det(Y(s))} ds.$$

Therefore,

$$(38) \quad \sqrt{\frac{\det(Y(0))}{\det(Y(T))}} = e^{-i\Theta_M},$$

where $\Theta_M := N_M \pi$ is the Maslov phase.

Notice that, the phases in real, time-dependent WKB theory, i.e., the Maslov indices, change discontinuously at caustics and are not always easy to determine, whereas in the Gaussian beam method the phase is found by continuously following the quantity $\det(Y(0))/\det(Y(t))$ and its square root along the orbit.

Proof. From (??), (??) and (??), we deduce

$$(39) \quad c_0(\hat{x}, x_3, \hat{y}) = \mathcal{O}\left(d(y, \Pi_{\hat{y}} \hat{\gamma})^3\right) \quad c_1(\hat{x}, x_3, \hat{y}) = \mathcal{O}\left(d(y, \Pi_{\hat{y}} \hat{\gamma})\right),$$

uniformly on $x \in \mathbb{T}$. By Proposition 1, we have $\Im \phi \geq C d(\hat{y}, \Pi_{\hat{y}} \hat{\gamma})^2$. Hence

$$d(\hat{y}, \Pi_{\hat{y}} \hat{\gamma})^m e^{i\phi/\epsilon} = \mathcal{O}(\epsilon^{m/2}),$$

which together with (??) and (??) produce the first three statements.

By (??), we have

$$(40) \quad \frac{d}{ds} \left[f_0(y(s)) \right] + \frac{1}{2} \left(\partial_y \cdot \partial_k E(\phi_y + \mu A(y), k_3) \right) \Big|_{y(s)} f_0(y(s)) + i \left(\dot{\theta}_b + \dot{\theta}_{rw} \right) f_0(y(s)) = 0.$$

We recall the $C(f_0, \partial_y f_0, \dots, \partial_y^\beta f_0) = 0$, when $\alpha = 0$. Next, by definition of $M(s)$, $B(s)$ and $C(s)$, we have :

$$\partial_y \cdot \partial_k E(\phi_y + \mu A(y)) \Big|_{y(s)} = \text{tr} \left(C(s) M(s) + B(s) \right).$$

From the first equation in (??), we deduce that $C(s)M(s)+B(s) = \dot{Y}(s)Y^{-1}(s)$. Combining this with the standard equality

$$\text{tr}(\dot{Y}(s)Y^{-1}(s)) = \frac{d}{ds} \ln(\det(Y(s)))$$

we obtain

$$(1/2)\partial_y \cdot \partial_k E(\phi_y + \mu A(y))|_{y(s)} = (1/2)\frac{d}{ds} \ln(\det(Y(s))),$$

which together with (??) yields

$$(41) \quad \frac{d}{ds} \left[f_0(\hat{y}(s)) \right] + \frac{1}{2} \frac{d}{ds} \ln(\det(Y(s))) f_0(\hat{y}(s)) + i \left(\dot{\theta}_b + \dot{\theta}_{rw} \right) f_0(\hat{y}(s)) = 0.$$

Now (??) follows from (??), (??), (??) and (??). We recall that $f_0(\hat{y}(0)) = 1$.

□

4. IMPLICATIONS

4.1. Generalized Onsager Relation. In physical space there is a motion in the y_3 -axis with velocity $\dot{y}_3(s) = \frac{\partial E}{\partial k_3}(k(s))$. Therefore, the orbits $\hat{\Gamma}(k_3)$ of the full hamiltonian in (??), (??) are helical, and do not support quasimodes, but their projections onto pseudo-momentum produce resonances (called "magnetic energy levels" in the physics literature). Onsager's key observation was that the magnetic energy levels determine $S(k_3)$ when it is extremal. Here we deduce that from the "resonance condition" that the phase of the beam must increase by an integer multiple of 2π when one goes around $\hat{\gamma}$. This means that $\phi(y(s))/\epsilon + \Theta(s)$ increases by a multiple of 2π , where $\Theta(s)$ represents the combined contributions of the Berry, Wilkinson-Rammal and Maslov phase shifts (see (??), (??) and Remark 3.)

Let us compute the change in ϕ around the periodic orbit $\hat{\gamma} = \hat{\gamma}(k_3, E_0, c)$. We denote T its period. From (??), $\phi_y(y(s)) = p(s)$. Since $\dot{p}_2(s) = 0$, it follows that

$$(42) \quad \dot{\phi}(y(s)) = p(s) \cdot \dot{y}(s) = p_1(s)\dot{y}_1(s) + p_2(s)\dot{y}_2(s) = \frac{1}{\mu} p_1(s)[\dot{p}_2(s) + \mu\dot{y}_1(s)] + p_2(0)\dot{y}_2(s).$$

Recall that $\gamma(k_3, E_0)$ will become $\hat{\gamma}(k_3, E_0, c)$ when one substitutes $k_1 = p_1$ and $k_2 = p_2 + \mu y_1$ and sets $y_2 = -p_1/\mu + c$. Combining this with the fact that $\int_0^T \dot{y}_2(s) ds = 0$, and using Green's theorem we obtain from (??)

$$\begin{aligned} \phi(y(T)) - \phi(y(0)) &= \int_0^T p(s)\dot{y}(s) ds = \int_0^T \frac{1}{\mu} p_1(s)[\dot{p}_2(s) + \mu\dot{y}_1(s)] ds \\ &= \frac{1}{\mu} \int_{\hat{\gamma}} k_1 dk_2 = \frac{S(k_3)}{\mu}. \end{aligned}$$

Combining the above equality with the resonance condition and using the fact that $\mu\hbar = e$, we obtain

$$(43) \quad \frac{\hbar}{e\epsilon} S(k_3) - \Theta = 2n\pi,$$

where $\Theta := \Theta_b + \Theta_{rw} + \Theta_M$ now stands for the change in $\Theta(s)$ around $\hat{\gamma}$, i.e.,

$$\Theta_b = -i \int_0^T \langle \Phi(\cdot, k(s)), \dot{\Phi}(\cdot, k(s)) \rangle ds = -i \int_{\hat{\gamma}} \langle \Phi(\cdot, k), \partial_k \Phi(\cdot, k) \rangle dk,$$

$$\Theta_{rw} = -\Im \int_0^T \langle (H_0(k(s)) - E) \frac{\partial \Phi}{\partial k_1}(\cdot, k(s)), \frac{\partial \Phi}{\partial k_2}(\cdot, k(s)) \rangle ds.$$

We recall that $\dot{\Phi}(\cdot, k(s)) = \dot{k}(s) \frac{\partial \Phi}{\partial k}(\cdot, k(s))$. Finally, according to (??), $\Theta_M = 0$ if N_M is even, and $\Theta_M = \pi$ if N_M is odd. Summing up, we obtain the generalized Onsager relation including the Berry, Ramal-Wilkinson, and Maslov phases :

Theorem 5. *Assume (H1-2), and let $S(k_3)$ denote the area in k -space enclosed by $\gamma(k_3, E_0)$. Therefore the quasi-classical quantization condition may be written in the form*

$$(44) \quad \frac{\hbar}{e\epsilon} S(k_3) = 2\pi(n + \gamma) + \Theta_b + \Theta_{rw},$$

where $\gamma = \frac{1}{2}$ or 0.

Magnetic Oscillation. The de Haas-van Alfvén effect is associated with closed curves γ in pseudo-momentum space formed by intersecting the Fermi surface with planes $k_3 = k_3^0$, where the (constant) magnetic field is parallel to the k_3 -axis. Not all choices for k_3^0 contribute to the de Haas-van Alfvén effect. Only the "extremal" values of k_3^0 , i.e. those for which $\frac{\partial S}{\partial k_3} = 0$, contribute. For each n Onsager's relation (??) determines a magnetic energy level by giving a relation between ϵ and $S(k_3)$. If $S(k_3^0)$ is extremal, as k_3 approaches k_3^0 smaller and smaller changes in ϵ are needed to satisfy Onsager's relation. Thus there is a peak in the density of magnetic energy levels at k_3^0 .

APPENDIX A

In this appendix, we recall some well known facts about the non-linear Riccati equation (??). For reader convenience we sketch the proofs. To construct a solution of (??), we start by choosing matrix solutions to the linear system

$$(A1) \quad \begin{cases} \dot{Y} = BY + CN \\ \dot{N} = -AY - B^T N. \end{cases}$$

Since A, B, C are well defined for all s , by linearity there exists a unique global solution $(Y(s), N(s))$ to the above system for any initial condition $(Y(0), N(0))$.

Let $G_1(s) = (Y^1(s), N^1(s))$ and $G_2(s) = (Y^2(s), N^2(s))$ be two vectors solutions of (??). We recall that

$$(A2) \quad \sigma(G_1(s), G_2(s)) = \sigma(G_1(0), G_2(0)).$$

Since $\overline{G_2(s)}$ is also a solution of (??), the complexified form $\sigma_{\mathbb{C}}$ is also constant in s , i.e.,

$$(A3) \quad \sigma_{\mathbb{C}}(G_1(s), G_2(s)) = \sigma(G_1(s), \overline{G_2(s)}) = \sigma_{\mathbb{C}}(G_1(0), G_2(0)).$$

Proposition 6. *Let M_0 be a symmetric matrix such that $\Im M_0$ is positive definite on the orthogonal complement of $\dot{y}(0) = (\dot{y}_1(0), \dot{y}_2(0))$, and $M_0 \dot{y}(0) = \dot{p}(0)$. Let $(Y(s), N(s))$ be the solution of (??) with initial condition $(Y(0), N(0)) = (I, M_0)$. We have*

- $(\dot{y}(s), \dot{p}(s)) = (Y(s)\dot{y}(0), N(s)\dot{y}(0))$.
- $Y(s)$ is invertible for all s .
- $M(s) := N(s)Y(s)^{-1}$ is a solution of the Riccati equation (??).
- $M(s)$ is a symmetric matrix for all $s \in \mathbb{R}$.
- The matrix $\Im M(s)$ is positive definite on the orthogonal complement of $\dot{y}(s) = (\dot{y}_1(s), \dot{y}_2(s))$.

Proof. The first claim follows from the fact that both $(Y(s)\dot{y}(0), N(s)\dot{y}(0))$ and $(\dot{y}(s), \dot{p}(s))$ are vector solutions of (??) as well as the fact that $(\dot{y}(0), \dot{p}(0)) = (Y(0)\dot{y}(0), N(0)\dot{y}(0))$.

Suppose that $Y(s)a = 0$ for some $a \in \mathbb{C}^2$. Since $(x(s), \xi(s)) := (Y(s)a, N(s)a)$ is a vector solution of (??), it follows from the constancy of complexified form $\sigma_{\mathbb{C}}$ that

$$\begin{aligned} 0 &= \sigma_{\mathbb{C}}((x(s), \xi(s)), (x(s), \xi(s))) = \sigma((x(0), \xi(0)), \overline{(x(0), \xi(0))}) \\ &= \overline{x(0)} \cdot \xi(0) - x(0) \cdot \overline{\xi(0)} = 2i\bar{a} \cdot \Im(M_0)a. \end{aligned}$$

By definition $\Im M_0$ is positive definite on the orthogonal complement of $\dot{y}(0)$. Combining this with the above equality we deduce that $a = \beta \dot{y}(0)$ for some $\beta \in \mathbb{C}$. Consequently,

$$0 = Y(s)a = \beta Y(s)\dot{y}(0) = \beta \dot{y}(s),$$

where we have used the first item. This gives the second item since $\dot{y}(s) \neq 0$ for all s , due to the assumption (H1).

To deal with the third item, notice that

$$\frac{d}{ds}(NY^{-1}) = \dot{N}Y^{-1} - NY^{-1}\dot{Y}Y^{-1},$$

which together with (??) yields

$$\frac{d}{ds}(NY^{-1}) = -A - B^T(NY^{-1}) - (NY^{-1})BY - (NY^{-1})C(NY^{-1}).$$

Hence $M(s) = NY^{-1}$ satisfies (??).

We pass to the fourth statement. Let $Y^i(s)$ (resp $N^i(s)$), $i = 1, 2$, denote the column vectors of $Y(s)$ (resp. $N(s)$), and let $G_i(s) = (Y^i(s), N^i(s))$. By construction of $M(s)$, we have $M(s)Y^i(s) = N^i(s)$.

From (??), we have

$$\begin{aligned}\sigma(G_i(s), G_j(s)) &= \sigma(G_i(0), G_j(0)) = Y^j(s) \cdot M(s)Y^i(s) - Y^i(s) \cdot M(s)Y^j(s) \\ &= Y^j(0) \cdot M(0)Y^i(0) - Y^i(0) \cdot M(0)Y^j(0).\end{aligned}$$

The right hand side of the last equation equals zero, since $M(0) = M_0$ is symmetric. Therefore, for all $s \in \mathbb{R}$,

$$Y^j(s) \cdot M(s)Y^i(s) = Y^i(s) \cdot M(s)Y^j(s).$$

Notice that $(Y^1(s), Y^2(s))$ is a basis in \mathbb{C}^2 , since $Y(s)$ is invertible for all s . Combining this with the above equality we deduce that $M(s)$ is symmetric.

The proof for the final item is almost identical to the proof of the second one, and relies on the conservation of the complexified form $\sigma_{\mathbb{C}}$.

□

REFERENCES

- [1] Arnaud, J. A., *Hamiltonian theory of beam mode propagation* in E. Wolf (ed), Progress in Optics XI, North Holland, 1973, pp. 249–304.
- [2] Ashcroft, N.W. and Mermin, N. D., *Solid State Physics*, Saunders College (1965).
- [3] Babich, V., *The higher-dimensional WKB method or ray method. its analogues and generalizations. In Partial Differential Equations V*. Springer, 1999, pp. 91–131.
- [4] Bellissard, J. and Rammal, R., *An algebraic semi-classical approach to Bloch electrons in a magnetic field*, J. Physique France 51 (1990), 1803.
- [5] Buslaev, V. S., *Semi-classical approximation for equations with periodic coefficients*, Russ. Math. Surv. 42 (1987), 97–125.
- [6] Dimassi, M., Guillot, J-C and Ralston, J., *Semi-Classical Asymptotics in Magnetic Bloch Bands*, J. Phys. A: Math. Gen. 35,(2002) pp. 7597–7605.
- [7] Dimassi, M., Guillot, J-C and Ralston, J., *Gaussian Beam Construction for Adiabatic Perturbations*. Mathematical Physics, Analysis and Geometry (2006), pp. 187–201.
- [8] Guillot, J.-C, Ralston, J., Trubowitz E., *Semi-classical methods in solid state physics*. Commun. Math. Phys. (1988), 116 401–15.
- [9] B. Helffer, J. Sjöstrand, *On diamagnetism and de Haas-van Alphen effect*. Annales de l' I. H. P., section A, tome 52, no 4 (1990), p. 303–375.
- [10] Hörmander, L., *Fourier integral operator I*, Acta Math. 127 (1971), 79 Y 183.
- [11] I. M. Lifshitz and Moisei I Kaganov, *Some Problems of the Electron Theory of Metals. I Classical and Quantum Theory of Electrons in Metals*. 1960 Sov. Physics Uspekhi 2, 831.
- [12] Liu, H., Runborg, O., and Tanushev, N. M. *Sobolev and max norm error estimates for Gaussian beam superpositions*. Commun. Math. Sci. 14, 7 (2016), 2037–2072.
- [13] Onsager, Lars, *Interpretation of the de Haas-van Alfvén Effect*, The Londo and Dublin Philosophical Mag. and J. of Science, (1952), pp. 1006–1008.
- [14] J. V. Ralston, *Approximate Eigenfunctions of the Laplacian..* J. Diff.Geometry Vol. 12 (1977), pp. 87–100.
- [15] J. V. Ralston, *On the Construction of Quasi-modes Associated with Stable Periodic Orbits*. Commun. in Math. Physics, vol. 51 (1976),pp. 219–242.
- [16] Peierls, R., *Zur Theorie des diamagnetismus von leitungselektronen*, Z. Phys. 80 (1933), 763 Y 791.
- [17] J. Sjöstrand, *Density of states oscillations for magnetic Schrödinger operators*. Mathematics in Science and Engineering Volume 186, 1992, Pages 295–345.

- [18] C. L. Siegel, J. Moser, *Lectures on Celestial Mechanics*. Berlin, Heidelberg, New York. Springer (1971).
- [19] Slater, J. C., *Electrons in perturbed periodic lattices*, *Phys. Rev.* 76 (1949), 1592–1600.
- [20] Sundaram, G. and Niu, Q., *Wave packet dynamics in slowly perturbed crystals: Gradient corrections and Berry phase effects*, *Phys. Rev. B* 59 (1999), 14915–14925.

MOUEZ DIMASSI, IMB (UMR-CNRS 5251), UNIVERSITÉ DE BORDEAUX, 351 COURS DE LA LIBÉRATION, 33405 TALENCE CEDEX, FRANCE

Email address: `mdimassi@u-bordeaux.fr`

J.-C. GUILLOT, UNIVERSITÉ D'AIX-MARSEILLE, CNRS, INSTITUT DE MATHÉMATIQUES DE MARSEILLE, UMR 7373, 13453 MARSEILLE CEDEX 13, FRANCE

Email address: `jcguillot@math.cnrs.fr`

J. RALSTON UNIVERSITY OF CALIFORNIA, LOS ANGELES, CA 90095, USA

Email address: `ralston@math.ucla.edu`