The Geometry of Algebraic Fermi Curves

D. Gieseker
H. Knörrer
E. Trubowitz

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D. Gieseker
Department of Mathematics
University of California
Los Angeles, California

H. Knörrer
E. Trubowitz
Department of Mathematics
Eidgenössische Technische Hochschule
Zürich, Switzerland

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Preface

Consider a discrete periodic Schrödinger operator $-\Delta + V$ acting on $\ell^2(\mathbb{Z}^2)$, where

$$\Delta\psi(m,n) = \psi(m+1,n) + \psi(m,n+1) + \psi(m-1,n) + \psi(m,n-1)$$

and V is real and periodic with respect to a sublattice $a\mathbb{Z} \oplus b\mathbb{Z}$. This book is devoted to the geometry of the associated Bloch (or spectral) variety

$$\begin{aligned} B = \quad & \{(\xi_1, \xi_2, \lambda) \in \mathbb{C}^* \times \mathbb{C}^* \times \mathbb{C} \mid \\ & \text{There is a non-trivial solution } \psi \text{ of} \\ & (-\Delta + V)(\psi) = \lambda\phi \text{ satisfying} \\ & \psi(m+a,n) = \xi_1\psi(m,n) \text{ and} \\ & \psi(m,n+b) = \xi_2\psi(m,n) \text{ for all} \\ & (m,n) \in \mathbb{Z}^2. \end{aligned}$$

Let $\pi : B \to \mathbb{C}$ be the projection and let $F_\lambda = \pi^{-1}(\lambda)$. The F_λ are called Fermi curves. For each real λ there is a holomorphic one form ω_λ on the algebraic curve F_λ and a cycle γ_λ in $H_1(F_\lambda, \mathbb{Z})$ such that the period $\int_{\gamma_\lambda} \omega_\lambda$ is the spectral density function of $-\Delta + V$ acting on $\ell^2(\mathbb{Z}^2)$ at λ. We exploit this connection between algebraic geometry of B and the spectral theory of the operator $-\Delta + V$ to study the inverse spectral problem.

A more detailed description of the contents of this book is contained in Chapters 1 and 3 as well as [GKT] and [P].

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1. The Periodic Schrödinger Operator and Electrons in a Crystal

Let us begin by recalling the static lattice approximation for electronic motion at low temperature in a pure, finite sample of a d-dimensional crystal.

The crystal structure is determined by specifying a lattice Γ in $\mathbf{R}^d$. For example, the common crystalline phase of iron is given by $\alpha e_1 \mathbf{Z} \oplus \alpha e_2 \mathbf{Z} \oplus \frac{\alpha}{2}(e_1 + e_2 + e_3)\mathbf{Z} \subset \mathbf{R}^3$, where $\alpha \approx 2.87\ A°$. At low temperature each atom has very little thermal energy and therefore moves in a small neighborhood of its equilibrium position at a lattice point. For this reason one makes the static lattice approximation in which a single ion is fixed at each lattice site.

The ions and conduction electrons interact through a two body potential u, so that

$$U(x) := \sum_{\gamma \in \Gamma} u(x - \gamma)$$

is the total potential for an electron at $x \in \mathbf{R}^d$ produced by the ions. Of course,

$$U(x + \gamma) = U(x), \quad \gamma \in \Gamma.$$

The conduction electrons also interact with each other via a two body potential, say W. Then, ignoring spin, the Hamiltonian operator for a system of N electrons in a pure, finite sample of size $L \in \mathbf{N}$ of the crystal is

$$\sum_{i=1}^{N} \Big(- \Delta_{x_i} + U(x_i) \Big) + \frac{1}{2} \sum_{i \neq j} W(x_i - x_j) \tag{1}$$

where x_i in $\mathbf{R}^d$ is the position of the i-th electron, and Δ_{x_i} denotes the Laplacian

$$\Delta_{x_i} := \sum_{j=1}^{d} \frac{\partial^2}{\partial x_i^{j2}}$$

with periodic boundary conditions on a fundamental cell of $L \cdot \Gamma$ centered at the origin; for example, $\left[-\frac{L}{2}, \frac{L}{2} \right]^d$ when $\Gamma = \mathbf{Z}^d$. Here, pure means that there is no static deviation from perfect periodicity; in particular, no ions are missing. The Hamiltonian operator acts on wave functions $\psi(x_1, \ldots, x_N)$ that are Fermionic*, by the Pauli exclusion principle, and periodic in each variable.

It is not feasible to analyse directly the spectrum of the interacting N-electron Hamiltonian. Therefore, another approximation is made. One imagines that by a suitable modification V of the periodic single electron potential U, the finite independent electron Hamiltonian

$$\sum_{i=1}^{N} -\Delta_{x_i} + V(x_i) \tag{2}$$

is, in important energy regimes, a good approximation to (1). For large samples, the boundary conditions become irrelevant for this model. The

*That is, $\psi(x_{\pi(1)}, \ldots, x_{\pi(N)}) = (-1)^{\sigma(\pi)} \psi(x_1, \ldots, x_N), \pi \in S_N$.

independent electron approximation of solid state physics is the limit of finite systems (2) as N and L tend to infinity with the density $\rho = \frac{N}{L^d}$ held fixed.

The independent electron approximation is remarkably successful and is, for instance, routinely used to calculate the electronic properties of metals. However, the only theoretical justification one has for ignoring electron-electron interactions in this way, is the quasiparticle picture of Landau, [AM].

Suppose $\psi_i(x), i = 1, \ldots, N$, satisfy the Schrödinger equation

$$(-\Delta + V(x))\psi_i = E_i\psi_i$$

with periodic boundary conditions

$$\psi(x + Le_j) = \psi(x)$$

$j = 1, \ldots, d$. Here, for simplicity, we consider the cubic lattice $\mathbf{Z}^d$. Then, by separation of variables

$$\psi(x_1, \ldots, x_N) = \det(\psi_i(x_j))$$

is a Fermionic N-electron wave function satisfying

$$\left(\sum_{j=1}^{N} -\Delta_{x_j} + V(x_j)\right)\psi = \left((\sum_{i=1}^{N} E_i)\psi\right)$$

and

$$\psi(x_1 + Le_j, x_2, \ldots, x_N) = \psi(x_1, \ldots, x_N),$$

$j = 1, \ldots, N$. Thus, from an orthogonal frame of eigenfunctions for the single particle operator $-\Delta + V(x)$ acting on $\mathbf{R}^d/L\mathbf{Z}^d$ one immediately constructs an orthonormal frame of Fermionic wave functions on $(\mathbf{R}^d/L\mathbf{Z}^d)^N$ for the N-particle operator $\left(\sum_{i=1}^{N} -\Delta_{x_i} + V(x_i)\right)$. Observe that the ground state energy of the N-particle operator is the sum of the first N eigenvalues of $-\Delta + V(x)$.

Let $V(x)$ be a sufficiently regular real-valued function on $\mathbf{R}^d/\Gamma$ (e.g. $V \in L^2(\mathbf{R}^d), d \leq 3$). For each k in $\mathbf{R}^d$ we consider the self-adjoint elliptic boundary value problem

$$(3)_k \qquad \begin{aligned} &(-\Delta + V(x))\psi = \lambda\psi \\ &\psi(x+\gamma) = e^{i\langle k,\gamma\rangle}\psi(x), \quad \gamma \in \Gamma. \end{aligned}$$

Let $E_n(k), n \geq 1$, be the n-th eigenvalue of $(3)_k$. It is easy to see that $E_n(k)$ is a continuous function of k that is periodic with respect to the lattice

$$\Gamma^{\#} = \{b \in \mathbf{R}^d \mid \langle b, \gamma\rangle \in 2\pi\mathbf{Z} \quad \text{for all} \quad \gamma \in \Gamma\}$$

dual to Γ. It is customary to refer to k as crystal momentum and to $E_n(k), n \geq 1$, as the n-th band function. The corresponding normalized eigenfunctions are denoted $\psi_n(x,k)$, and are called Bloch eigenfunctions.

A hyperplane in $\mathbf{R}^d$ perpendicularly bisecting a dual lattice vector $b \in \Gamma^{\#}$ is called a Bragg hyperplane. The set of all points in $\mathbf{R}^d$ that can be reached from the origin without crossing any Bragg hyperplane is called the first Brillouin zone of $\Gamma^{\#}$. Similarly, the set of all points that can be reached by crossing $n-1$ but not n Bragg hyperplanes is called the n-th Brillouin zone. Each Brillouin zone is a fundamental region for $\Gamma^{\#}$. Since the band functions are periodic with respect to $\Gamma^{\#}$ we may plot $E_1(k)$ over the first Brillouin zone, E_2 over the second and so on, to obtain a function $E(k)$ defined on $\mathbf{R}^d$ called the energy-crystal momentum dispersion relation. In the same way, one defines $\psi(x,k)$, $k \in \mathbf{R}^d$, by plotting $\psi_1(x,k)$ over the first Brillouin zone and so on.

Once again, for the sake of convenience, assume that the underlying lattice Γ is $\mathbf{Z}^d$. Suppose that $k \in \frac{2\pi}{L}\mathbf{Z}^d$. Then any solution of $(3)_k$ satisfies

$$\psi(x + Le_j) = \psi(x), j = 1, \ldots, d.$$

It is easy to see that the converse is also true. Thus, the spectrum of $-\Delta + V(x)$ acting on $L^2(\mathbf{R}^d/L\mathbf{Z}^d)$ is

$$\left\{E(k) \mid k \in \frac{2\pi}{L}\mathbf{Z}^d\right\}.$$

Let $k_1, \ldots, k_N \in \frac{2\pi}{L}\mathbf{Z}^d$ be the crystal momenta such that

$$E(k_1) \leq \cdots \leq E(k_N)$$