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Autor: Moroz, Alexander
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Universal dependence of eigenvectors of tight-binding models on Bloch momenta

ALEXANDER MOROZ

Institute of Physics ČSAV, Na Slovance 2

CS-180 40 Prague 8, Czechoslovakia

Abstract. A connection of a variety of tight-binding models of noninteracting electrons in a rational magnetic field with theta functions is established. Eigenvectors of the tight-binding models are shown to have a universal dependence on Bloch momenta.

In what follows the Landau gauge $\vec{A} = B(-y, 0, 0)$ and, for definiteness, a rectangular lattice is assumed, $\vec{a}_1$ and $\vec{a}_2$ being primitive vectors of lattice translations in x and y direction, respectively. We shall consider the tight-binding Hamiltonian $\mathcal{H}$ [1,2],

$$\mathcal{H} = t_1(S_{\vec{a}_1} + S_{\vec{a}_1}^* + S_{\vec{a}_2} + S_{\vec{a}_2}^*) + \dots, \quad (1)$$

where $S_{\pm\vec{a}_i}$ ($S_{-\vec{a}_i} = S_{\vec{a}_i}^*$) is a shift operator, $S_{\pm\vec{a}_j} = e^{\pm \frac{i}{\hbar} \vec{a}_j \cdot m \hat{v}_j}$, operators $\hat{v}_j$, $j = 1, 2$, being components of the standard velocity operator, and $\dots$ in (1) stand for integer powers j of the shift operators multiplied by a corresponding overlap integral t_j and describing next-nearest-neighbour hopping, etc. The spectrum of $\mathcal{H}$ strongly depends on a parameter $\alpha = \Phi/\Phi_0$, Φ and $\Phi_0 = hc/e$ being the magnetic flux through an elementary plaquette and the flux quantum, respectively, and it is symmetric under $\alpha \rightarrow \alpha + 1$ [2]. In a magnetic field the translation operators are replaced by the operators of magnetic translations $T_{\vec{a}_j}$, $j = 1, 2$, generated by the spatial parity transformed components of the operator $m\vec{v}/\hbar$, $\vec{v}$ being velocity operator. In a rational magnetic field $\alpha = p/q$, p and q being relative prime integers, the spectrum can be classified by irreducible representations of the magnetic group generated by $T_{\vec{a}_1}$ and $T_{\vec{a}_2}^q$. $\mathcal{H}$ however commutes with any power of the magnetic translation operators, i.e., with the full Heisenberg group [3]. $\mathcal{H}$ leads on a finite difference equation (called in the case of the nearest-neighbour tight-binding model as the Harper equation [1,2]) and hence it determines an eigenfunction ψ at discrete set of points only. In what follows we shall not confine ourselves to the lattice sites only and we shall consider the Harper equation associated with any point (x_0, y_0) of the primitive cell. The crucial observation is that the values of ψ on a sublattice defined by

translations by q lattice spacings in x direction do determine an element of V , the Hilbert space of entire functions in the complex variable $z = X + iY$, where $X = x/a_1$ and $Y = \alpha y/2\pi a_2$. For any $f \in V$ we shall consider the function g ,

$$g^{k_1 k_2}(x, y) = e^{i\vec{k}\vec{r}} e^{-y^2 \alpha^2 / 2a_2^2} f(x, y). \quad (2)$$

The functions g^s are bounded functions on the Riemann sphere and form the Hilbert space W with the usual L^2 scalar product. $\mathcal{H}$ then acts in the subspace W_q of W generated by $g_\ell = e^{i\vec{k}\vec{r}} e^{-y^2 \alpha^2 / 2a_2^2} \Theta_\ell$, Θ_ℓ being the Jacobi theta function with a rational characteristics ℓ [4],

$$\Theta_\ell(x, y) = \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{1}{2}(n + \ell\alpha)^2 + 2\pi i(n + \ell\alpha)\left(\frac{x}{a_1} + i\alpha\frac{y}{2\pi a_2}\right)\right\}. \quad (3)$$

They are written in a form which enables to discuss a limit when $q \rightarrow \infty$, i.e., irrational α . In virtue of the properties of g_ℓ under lattice translations,

$$\begin{aligned} g_\ell(x \pm a_1, y) &= e^{ik_1 a_1} e^{\pm 2\ell\pi i \alpha} g_\ell(x, y) \\ g_\ell(x, y \pm a_2) &= e^{ik_2 a_2} e^{\mp 2\pi i \alpha x/a_1} g_{\ell \pm 1}(x, y). \end{aligned} \quad (4)$$

one finds that the components $d_\ell(k_1, k_2)$ of an eigenvector $\vec{d} = \sum_\ell d_\ell(k_1, k_2) \tilde{g}_{\ell, (x_0, y_0)}^{k_1 k_2}(x, y)$, $\tilde{g}_\ell$ being suitable rotated g_ℓ , depend on the Bloch momenta as follows,

$$\begin{aligned} d_\ell(k_1 + 2\pi\alpha\sigma_2/a_1, k_2 + 2\pi\alpha\sigma_1/a_2) = \\ \sum_{s=0}^{q-1} d_s(k_1, k_2) \langle \tilde{g}_s^{k_1 k_2}(x, y) | \tilde{g}_\ell^{k_1 + 2\pi\alpha\sigma_2/a_1, k_2}(x + \sigma_1 a_1, y + \sigma_2 a_2) \rangle_W. \end{aligned} \quad (5)$$

Thus the problem of diagonalization of the tight-binding models can be reduced to the problem of finding initial conditions for the matrix on the r.h.s. of (5) [3].

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