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Autor(en): **Moroz, Alexander**

Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **65 (1992)**

Heft 2-3

PDF erstellt am: **25.09.2024**

Persistenter Link: https://doi.org/10.5169/seals-116437

Universal dependence of eigenvectors of tight-binding models on Bloch momenta

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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 definitness, a rectangulár 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],

$$\mathcal{H} = t_1(S_{\vec{a_1}} + S^*_{\vec{a_1}} + S_{\vec{a_2}} + S^*_{\vec{a_2}}) + \ldots, \tag{1}$$

where $S_{\pm\vec{a_l}}$ $(S_{-\vec{a_l}} = S^*_{\vec{a_l}})$ is a shift operator, $S_{\pm\vec{a_j}} = e^{\pm\frac{i}{\hbar}a_j m\hat{v}_j}$, operators $\hat{v}_j$, $j = 1,2$, being components of the standard velocity operator, and ... in (1) stand for integer powers j of the shift opertors 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 $\alpha = \Phi/\Phi_o$, Φ and $\Phi_o = hc/e$ being the magnetic flux through an elementary plaquette and the flux quantum, respectively, and it is symmetric under $\alpha \to \alpha + 1$ [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 $T^q_{\vec{a_2}}$}. $\mathcal{H}$ however commutes with any power of the magnetic translation operators, i.e., with the full Heiseberg group [3]. $\mathcal{H}$ leads on a finite diference 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_o, y_o) 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,

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

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],

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

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

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

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

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

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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