

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

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

Objektyp: **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>

Nutzungsbedingungen

Die ETH-Bibliothek ist Anbieterin der digitalisierten Zeitschriften. Sie besitzt keine Urheberrechte an den Inhalten der Zeitschriften. Die Rechte liegen in der Regel bei den Herausgebern.

Die auf der Plattform e-periodica veröffentlichten Dokumente stehen für nicht-kommerzielle Zwecke in Lehre und Forschung sowie für die private Nutzung frei zur Verfügung. Einzelne Dateien oder Ausdrucke aus diesem Angebot können zusammen mit diesen Nutzungsbedingungen und den korrekten Herkunftsbezeichnungen weitergegeben werden.

Das Veröffentlichen von Bildern in Print- und Online-Publikationen ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. Die systematische Speicherung von Teilen des elektronischen Angebots auf anderen Servern bedarf ebenfalls des schriftlichen Einverständnisses der Rechteinhaber.

Haftungsausschluss

Alle Angaben erfolgen ohne Gewähr für Vollständigkeit oder Richtigkeit. Es wird keine Haftung übernommen für Schäden durch die Verwendung von Informationen aus diesem Online-Angebot oder durch das Fehlen von Informationen. Dies gilt auch für Inhalte Dritter, die über dieses Angebot zugänglich sind.

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 $S_{\pm\vec{a}_l}$ ($S_{-\vec{a}_l} = S_{\vec{a}_l}^*$) 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 \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 Heiseberg 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,

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

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

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

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].

References

- [1] P. G. Harper, Proc. Phys. Soc. Lond. A **68**, 874 (1955).
- [2] D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976).
- [3] A. Moroz, MPI/Ph 991-22 and Prague preprint PRA-HEP 91/6.
- [4] D. Mumford, *Tata lectures on theta I* (Birkhäuser, Stuttgart, 1982), Ch.1, §3; D. Mumford, M. Nori, and P. Norman, *Tata lectures on theta III* (in print).