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Two-scale relations in one-dimensional crystals and wavelets

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Abstract. We present a complete analysis of scale transformation of the Bloch functions and the Wannier functions in one-dimensional lattices, when a cell twice as large as the primitive cell is taken as the periodic unit. We obtain the Wannier functions for a free electron imposing an artificial periodicity and show that the Wannier functions satisfy the properties of the wavelets and wavelet packets of the multi-resolution analysis. We show that the coefficients appearing in the scale transformation of the Wannier functions for a free electron also serve as the expansion coefficients for the scale transformation of the Bloch functions and the Wannier functions in general one-dimensional lattices. Finally, we argue the importance of the translational symmetry based on the minimal primitive cell in determining the Wannier functions.

1. Introduction

It is well known that one-electron states in periodic crystals can be completely described by Bloch's theorem. Because of the translational symmetry, the Hamiltonian of a periodic system commutes with translation operators generated by the Bravais lattice and the eigenfunctions, Bloch functions, of the Hamiltonian can be represented by the product of a plane wave whose wavevector lies in the first Brillouin zone and a periodic function of the Bravais lattice [1].

The period of a crystal is usually taken as the shortest of any possible period. However, we can always view a periodic system with period a as a system with period $2a$ or any integer multiples of a. We call this transformation 'inflation' or renormalization of the unit cell. The inflation transformation can be considered as a kind of symmetry operation of the periodic system. It is known that the reciprocal lattice does not essentially change under the inflation if one takes account of the structure factor. In fact, the scattering function $I^{(a)}(k)$ for a one-dimensional lattice with period a is given by

$$I^{(a)}(k) \equiv \frac{a}{2\pi}\sum_{m=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kam} = \sum_{l=-\infty}^{\infty} \delta\left(k - \frac{2\pi}{a}l\right). \tag{1.1}$$

If we view the same system as possessing period $2a$, the scattering function is expressed with the structure factor $1 + \mathrm{e}^{\mathrm{i}ka}$ as

$$\begin{aligned} I^{(2a)}(k) &= \frac{a}{2\pi}\sum_{m=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}ka2m}\left(1 + \mathrm{e}^{\mathrm{i}ka}\right) \\ &= \sum_{l=-\infty}^{\infty} \delta\left(k - \frac{\pi}{a}l\right)\left(1 + \mathrm{e}^{\mathrm{i}ka}\right). \end{aligned} \tag{1.2}$$

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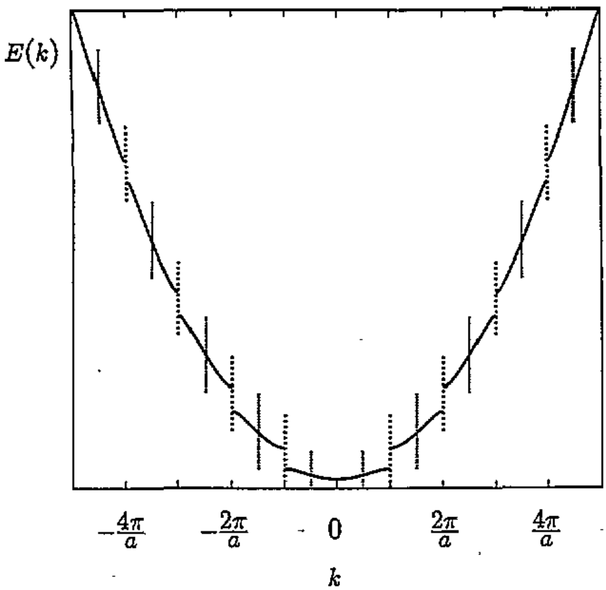

Figure 1. Electronic energy levels in a one-dimensional lattice versus wavevector k are shown schematically in an extended-zone scheme. The Bragg planes corresponding to lattice constant a are denoted by broken lines, and the Bragg planes corresponding to lattice constant $2a$ are denoted by dotted lines. Note there are no band gaps at the fictitious Blagg planes.

Obviously at $k = (2l+1)\pi/a$, where is l an integer, the structure factor vanishes, and the scattering function $I^{(2a)}(k)$ becomes identical to $I^{(a)}(k)$. It is also clear that when the unit cell is inflated, the energy bands are folded at the new Bragg planes though band gaps do not appear at the new Bragg planes because of the same reason as above (see figure 1). However, it is not trivial how the Bloch functions and the Wannier functions are transformed under the inflation. In this paper, we give a complete analysis to this question for one-dimensional periodic lattices. In particular, we show that the Wannier functions for a free electron in one dimension are the wavelets and wavelet packets known in the multi-resolution analysis.

Consider an electron in a one-dimensional periodic lattice, whose Hamiltonian is given by

$$H(x;a) = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + U(x) \tag{1.3}$$

where M is the mass of the electron and the periodic potential energy $U(x)$ satisfies

$$U(x+a) = U(x).$$

If we introduce a scaled coordinate

$$\bar{x}^{(1)} = \frac{x}{a}$$

then the scaled Hamiltonian is given by

$$\bar{H}^{(1)}(\bar{x}^{(1)}) \equiv \frac{2Ma^2}{\hbar^2}H(a\bar{x}^{(1)};a) = -\frac{\mathrm{d}^2}{\mathrm{d}\bar{x}^{(1)2}} + \bar{U}^{(1)}(\bar{x}^{(1)}) \tag{1.4}$$

where

$$\bar{U}^{(1)}(\bar{x}^{(1)}) = \frac{2Ma^2}{\hbar^2}U(x)$$

which has a period of unit length. Suppose we consider the period of this system to be $2a$, then the scaled Hamiltonian (scaled as $\bar{x}^{(2)} = x/2a$) is

$$\bar{H}^{(2)}(\bar{x}^{(2)}) \equiv \frac{2M(2a)^2}{\hbar^2} H(2a\bar{x}^{(2)}; a) = -\frac{\mathrm{d}^2}{\mathrm{d}\bar{x}^{(2)2}} + \bar{U}^{(2)}(\bar{x}^{(2)}) \tag{1.5}$$

where the scaled potential energy is given by

$$\bar{U}^{(2)}(\bar{x}^{(2)}) = \frac{2M(2a)^2}{\hbar^2} U(x)$$

which also has a period of unit length. If $\bar{U}^{(1)}(x) = \bar{U}^{(2)}(x)$ holds, then the inflation is a symmetry operation of the Hamiltonian and we expect a certain symmetry in the Bloch functions. When $\bar{U}^{(1)}(x) \neq \bar{U}^{(2)}(x)$, which holds in most crystals, the inflation transformation is not a symmetry operation to the Hamiltonian. However, we can still find definite relations among differently scaled eigenfunctions.

Throughout this paper we focus on inflation by a factor 2, that is, scaling by a factor 2 which we call a 'two-scale by factor 2' or simply 'two-scale'. It should be emphasized that a similar discussion holds for any other integer scaling factor.

In section 2, we briefly review the Bloch representation of the eigenfunctions for a one-dimensional periodic system and Wannier functions. In section 3, we discuss the case where the relation

$$\bar{H}^{(1)}(x) = \bar{H}^{(2)}(x) \tag{1.6}$$

holds and the scaling transformation is a symmetry operation. This symmetry exists when the potential energy is identically zero, namely, for a free electron. We can obtain Wannier functions directly (Wannier functions of a free electron), and we derive the two-scale relations and decomposition relations among differently scaled Wannier functions by direct calculation of their inner product. We show that Wannier functions of the zeroth and first bands form the scaling functions and wavelets, respectively, and we explain the correspondence between these two-scale relations and the wavelet analysis. In section 4, we discuss two-scale relations when the potential energy is not identically zero. We show that the two-scale relations of the Bloch functions found for a free electron can also be extended to this case, though the Wannier functions cannot be related to wavelets. In section 5, we apply the present analysis to a model system consisting of infinite potential barriers placed periodically. We argue the importance of the translational symmetry of the whole system in dealing with the inflation transformation. We give a brief summary and comments in section 6.

2. Bloch's theorem and Wannier functions

In the following discussion, we denote the set of integers by

$$\mathbb{Z} = \{\ldots, -1, 0, 1, \ldots\} \qquad \mathbb{Z}_+ = \{0, 1, 2, 3, \ldots\}$$

and the space of measurable functions f by $L^2(\mathbb{R})$, where f is defined on the real line $\mathbb{R}$, which satisfies

$$\langle f(\cdot), f(\cdot)\rangle < \infty$$

with the inner product

$$\langle f(\cdot), g(\cdot)\rangle = \int_{-\infty}^{\infty} f^*(x) g(x)\,\mathrm{d}x\,.$$

We may drop $(\cdot)$ in the notation when it is apparent.

In one-dimensional crystals with lattice constant a, the stationary Schrödinger equation is

$$H(x;a)\psi_{n,k}^{(a)}(x) = \varepsilon_{n,k}^{(a)}\psi_{n,k}^{(a)}(x) \tag{2.1}$$

$$\pi n \leqslant |k|a < \pi(n+1) \qquad n \in \mathbb{Z}_+$$

and its eigenfunction $\psi_{n,k}^{(a)}(x)$, the Bloch function, is written as the product of a plane wave and a periodic function of the lattice,

$$\psi_{n,k}^{(a)}(x) = \mathrm{e}^{\mathrm{i}kx}u_{n,k}^{(a)}(x) \qquad\qquad u_{n,k}^{(a)}(x+a) = u_{n,k}^{(a)}(x)\,. \tag{2.2}$$

Here n is the band index and we used the extended zone scheme, where the energy bands are represented as a single-valued function of k. This choice of the scheme will make it easier to find the correspondence between crystals and systems without the translational symmetry of the Bravais lattice. The Bloch functions satisfy the normalization condition

$$\langle\psi_{n',k'}^{(a)}, \psi_{n,k}^{(a)}\rangle = \delta_{n',n}\delta(k'-k)\,. \tag{2.3}$$

The Bloch function can be written as a linear combination of Wannier functions [1];

$$\psi_{n,k}^{(a)}(x) = \sqrt{\frac{a}{2\pi}}\sum_{m=-\infty}^{\infty}\phi_n^{(a)}(x-am)\mathrm{e}^{\mathrm{i}kam} \tag{2.4}$$

where the Wannier function $\phi_n^{(a)}(x)$ of the nth band is localized at $x=0$. Conversely, the Wannier function of the nth band can be represented as the superposition of the Bloch functions (the inversion formula of Fourier coefficients);

$$\phi_n^{(a)}(x-am) = \sqrt{\frac{a}{2\pi}}\int_{-\frac{\pi}{a}(n+1)}^{-\frac{\pi}{a}n}\psi_{n,k}^{(a)}(x)\mathrm{e}^{-\mathrm{i}kam}\,\mathrm{d}k + \sqrt{\frac{a}{2\pi}}\int_{\frac{\pi}{a}n}^{\frac{\pi}{a}(n+1)}\psi_{n,k}^{(a)}(x)\mathrm{e}^{-\mathrm{i}kam}\,\mathrm{d}k \tag{2.5}$$

where the integration range is the nth Brillouin zone. Note that the integration can be performed for any Brillouin zone, since the Bloch function is a periodic function in k-space. The prefactor $\sqrt{a/2\pi}$ in (2.5) ensures the normalization of the Wannier function

$$\langle\phi_{n_1}^{(a)}(\cdot - am_1), \phi_{n_2}^{(a)}(\cdot - am_2)\rangle = \delta_{n_1,n_2}\delta_{m_1,m_2}\,. \tag{2.6}$$

Since the complete set of Bloch functions is written as a unitary transformation of the Wannier functions, the Wannier functions $\phi_n^{(a)}(x-am)$ for $n \in \mathbb{Z}_+$ and $m \in \mathbb{Z}$ form an orthonormal complete set.

3. Wannier functions for a free electron and wavelets

We consider a free electron in one dimension whose Hamiltonian is

$$H(x;a) = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,. \tag{3.1}$$

We impose an artificial periodicity of period a. Since this Hamiltonian satisfies (1.6), the scaling transformation is a symmetry operation for this system. The solution of the one-electron Schrödinger equation is given by

$$\psi_{n,k}^{(a)}(x) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}kx} \tag{3.2}$$

$$\varepsilon_{n,k}^{(a)} = \frac{\hbar^2k^2}{2M} \qquad \pi n \leqslant |k|a < \pi(n+1) \tag{3.3}$$

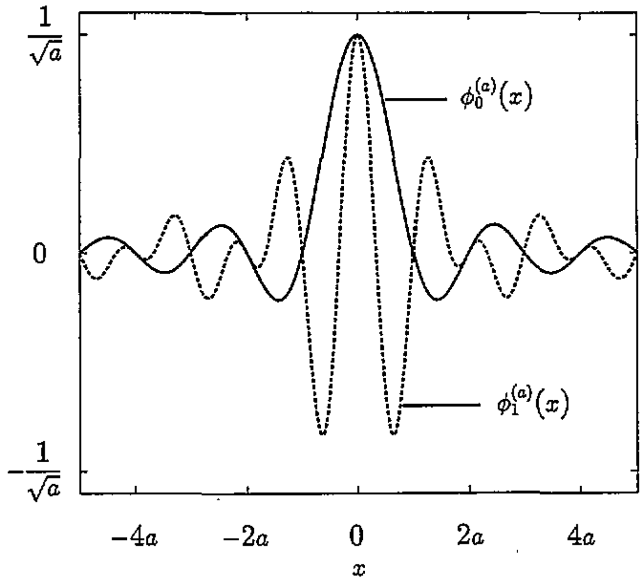

Figure 2. The Wannier functions around the origin of the first two energy bands for a free electron in one dimension. The Wannier functions of the higher bands behave similarly with more oscillation.

for all $n \in \mathbb{Z}_+$. This solution, of course, agrees with the solution for the system without the artificial periodicity. From equations (2.5) and (3.2), the Wannier functions for a free electron can immediately be obtained:

$$\phi_n^{(a)}(x-am) = \frac{\sqrt{a}}{\pi}\frac{1}{x-am}\left\{\sin\left[\frac{\pi}{a}(n+1)(x-am)\right] - \sin\left[\frac{\pi}{a}n(x-am)\right]\right\}. \tag{3.4}$$

This Wannier function is localized at $x = am$ and decays hyperbolically with oscillation as $|x-am|$ is increased. We show the Wannier function $\phi_n^{(a)}(x)$ for $n = 0$ and 1 in figure 2. In passing, in figure 3 we show the Fourier transform of $\phi_n^{(a)}(x)$:

$$\begin{aligned}\widehat{\phi_n}^{(a)}(k) &= \int_{-\infty}^{\infty} \mathrm{d}x\, \phi_n^{(a)}(x)\mathrm{e}^{-ikx} \\ &= \begin{cases} \sqrt{a} & n\pi \leqslant |k|a < (n+1)\pi \\ 0 & \text{otherwise}. \end{cases}\end{aligned} \tag{3.5}$$

In particular, we note that the support of $\widehat{\phi_0}^{(a)}(k)$ is $|k| \leqslant \pi/a$.

3.1. Two-scale relations of the Wannier functions for a free electron

We can construct the Wannier function for a free electron using any lattice constant. We consider the Wannier function $\phi_n^{(2a)}$ for lattice constant $2a$. It is straightforward to show the following two properties. First, $\phi_n^{(2a)}(x)$ and $\phi_n^{(a)}(x)$ satisfy

$$\sqrt{2}\phi_n^{(2a)}(2x-2am) = \phi_n^{(a)}(x-am). \tag{3.6}$$

The left-hand side denotes the Wannier function (times $\sqrt{2}$) for a free electron in a one-dimensional lattice with lattice constant $2a$ compressed by a factor 2 towards the origin, which is localized at $2am$ before the compression and at am after the compression. Note that $\phi_n^{(2a)}(x)$ satisfies the normalization condition

$$\langle \phi_{n_1}^{(2a)}(\cdot - 2am_1), \phi_{n_2}^{(2a)}(\cdot - 2am_2)\rangle = \delta_{n_1,n_2}\delta_{m_1,m_2}. \tag{3.7}$$

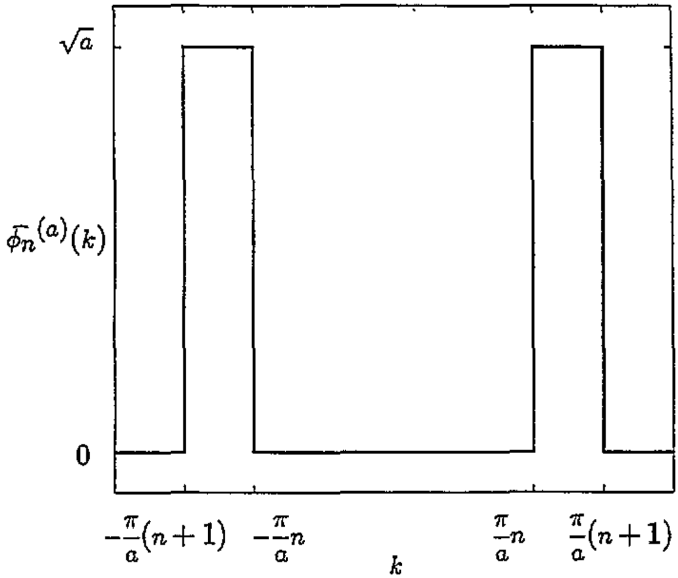

Figure 3. The Fourier transform of the Wannier function of the nth band for a free electron in one dimension.

Secondly, the inner product between the Wannier functions $\phi_n^{(a)}(x)$ and $\phi_{n'}^{(2a)}(x)$ does not depend on parameter a, namely, we can show

$$
\begin{aligned}
\langle\phi_{2n}^{(a)}(\cdot - am_1), \phi_{n'}^{(2a)}(\cdot - 2am_2)\rangle &= \begin{cases} p_{m_1-2m_2} & \text{for} \quad n' = 4n \\ q_{m_1-2m_2} & \text{for} \quad n' = 4n+1 \\ 0 & \text{otherwise} \end{cases} \\
\langle\phi_{2n+1}^{(a)}(\cdot - am_1), \phi_{n'}^{(2a)}(\cdot - 2am_2)\rangle &= \begin{cases} p_{m_1-2m_2} & \text{for} \quad n' = 4n+3 \\ q_{m_1-2m_2} & \text{for} \quad n' = 4n+2 \\ 0 & \text{otherwise} \end{cases}
\end{aligned}
\tag{3.8}
$$

where

$$
p_m = \frac{\sqrt{2}}{\pi}\frac{\sin(\pi m/2)}{m} \tag{3.9a}
$$

$$
q_m = \begin{cases} -\dfrac{\sqrt{2}}{\pi}\dfrac{\sin(\pi m/2)}{m} & \text{for} \quad m \neq 0 \\ \dfrac{1}{\sqrt{2}} & \text{for} \quad m = 0\,. \end{cases} \tag{3.9b}
$$

Here the Parseval identity has been used to derive (3.9a) and (3.9b). The sequences $\{p_m\}$ and $\{q_m\}$ play important roles in the following discussion.

Considering the orthogonal decomposition of the space $L^2(\mathbb{R})$ (see appendix A), and using the relation (3.6), we can derive the following two-scale relations of the Wannier functions

$$
\phi_{4n}^{(a)}(x - am_2) = \sum_{m_1=-\infty}^{\infty} p_{m_1-2m_2}\sqrt{2}\phi_{2n}^{(a)}(2x - am_1) \tag{3.10a}
$$

$$
\phi_{4n+1}^{(a)}(x - am_2) = \sum_{m_1=-\infty}^{\infty} q_{m_1-2m_2}\sqrt{2}\phi_{2n}^{(a)}(2x - am_1) \tag{3.10b}
$$

$$\phi^{(a)}_{4n+3}(x-am_2)=\sum_{m_1=-\infty}^{\infty}p_{m_1-2m_2}\sqrt{2}\phi^{(a)}_{2n+1}(2x-am_1) \tag{3.10c}$$

$$\phi^{(a)}_{4n+2}(x-am_2)=\sum_{m_1=-\infty}^{\infty}q_{m_1-2m_2}\sqrt{2}\phi^{(a)}_{2n+1}(2x-am_1) \tag{3.10d}$$

for all $m_2 \in \mathbb{Z}$. For example, equation (3.10a) denotes that the Wannier function $\phi^{(a)}_{4n}(x)$ for the 4nth band can be expressed as a linear combination of the Wannier functions for the 2nth band compressed toward the origin by factor 2 (see figure 4). equations (3.10b)–(3.10d) have similar meanings.

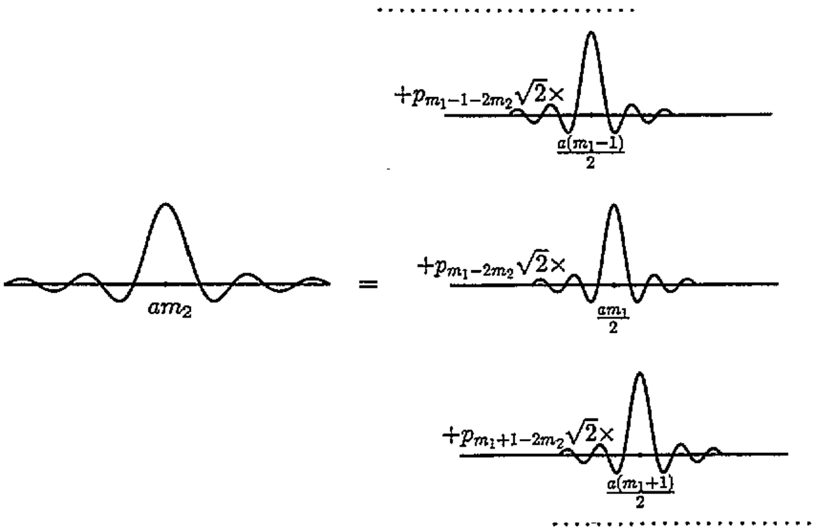

Figure 4. The two-scale relations between $\phi^{(2a)}_n(x)$ and $\phi^{(a)}_{n'}(x)$ are shown schematically.

The inverse transformation of equations (3.10a)–(3.10d) is given by the decomposition relations

$$\sqrt{2}\phi^{(a)}_{2n}(2x-am_1)=\sum_{m_2=-\infty}^{\infty}p^*_{m_1-2m_2}\phi^{(a)}_{4n}(x-am_2)+\sum_{m_2=-\infty}^{\infty}q^*_{m_1-2m_2}\phi^{(a)}_{4n+1}(x-am_2) \tag{3.11a}$$

$$\sqrt{2}\phi^{(a)}_{2n+1}(2x-am_1)=\sum_{m_2=-\infty}^{\infty}p^*_{m_1-2m_2}\phi^{(a)}_{4n+3}(x-am_2)+\sum_{m_2=-\infty}^{\infty}q^*_{m_1-2m_2}\phi^{(a)}_{4n+2}(x-am_2) \tag{3.11b}$$

for all $m_1 \in \mathbb{Z}$. Here we have used complex conjugates in the coefficients, although $\{p_m\}$ and $\{q_m\}$ are real, to clearly indicate that the decomposition relations (3.11a) and (3.11b) are the inverse transformations of two-scale relations (3.10a)– (3.10d). The coefficients $\{p_m\}$ and $\{q_m\}$ are elements of a unitary matrix for the inflation transformation which satisfy the following orthogonality relations (see also equations (A.9)–(A.12) in appendix A).

$$\sum_{m=-\infty}^{\infty}p^*_{m-2m_1}p_{m-2m_2}=\delta_{m_1,m_2} \tag{3.12a}$$

$$\sum_{m=-\infty}^{\infty} q^*_{m-2m_1} q_{m-2m_2} = \delta_{m_1,m_2} \tag{3.12b}$$

$$\sum_{m=-\infty}^{\infty} p^*_{m-2m_1} q_{m-2m_2} = 0 \tag{3.12c}$$

$$\sum_{m=-\infty}^{\infty} \{p^*_{m_1-2m} p_{m_2-2m} + q^*_{m_1-2m} q_{m_2-2m}\} = \delta_{m_1,m_2} . \tag{3.12d}$$

Equations (3.10*a*)–(3.10*d*) and (3.11*a*), (3.11*b*) define the renormalization relation of the Wannier functions for a free electron with respect to the inflation of the unit cell. These relations form the main properties of the wavelet analysis as we explain in the next subsection.

3.2. *Wannier functions for a free electron as wavelets*

From the renormalization relations of the Wannier functions for band index $n = 0$ and $n = 1$, we find the following important results. For $n = 0$, equations (3.10*a*), (3.10*b*) and (3.11*a*) become

$$\phi_0^{(a)}(x - am_2) = \sum_{m_1=-\infty}^{\infty} p_{m_1-2m_2} \sqrt{2} \phi_0^{(a)}(2x - am_1) \tag{3.13a}$$

$$\phi_1^{(a)}(x - am_2) = \sum_{m_1=-\infty}^{\infty} q_{m_1-2m_2} \sqrt{2} \phi_0^{(a)}(2x - am_1) \tag{3.13b}$$

$$\sqrt{2} \phi_0^{(a)}(2x - am_1) = \sum_{m_2=-\infty}^{\infty} p^*_{m_1-2m_2} \phi_0^{(a)}(x - am_2) + \sum_{m_2=-\infty}^{\infty} q^*_{m_1-2m_2} \phi_1^{(a)}(x - am_2) . \tag{3.14}$$

Obviously equations (3.13*a*)–(3.14) are closed relations among $\phi_0^{(a)}$ and $\phi_1^{(a)}$. The linear spans of these basis functions form subspaces of $L^2(\mathbb{R})$ such that

$$U_0^{(a)} = \mathrm{clos}_{L^2(\mathbb{R})} \langle \phi_0^{(a)}(\cdot - am) : m \in \mathbb{Z} \rangle \tag{3.15}$$

$$U_1^{(a)} = \mathrm{clos}_{L^2(\mathbb{R})} \langle \phi_1^{(a)}(\cdot - am) : m \in \mathbb{Z} \rangle \tag{3.16}$$

and from equation (A.4) of appendix A the space $U_0^{(a)}$ is shown to be decomposed as

$$\begin{aligned} U_0^{(a)} &= U_0^{(2a)} \oplus U_1^{(2a)} \\ &= U_0^{(4a)} \oplus U_1^{(4a)} \oplus U_1^{(2a)} \\ &= \cdots \oplus U_1^{(8a)} \oplus U_1^{(4a)} \oplus U_1^{(2a)} . \end{aligned} \tag{3.17}$$

On the other hand, we can start this decomposition of the subspace from any a, for example, $U_0^{(a/2)} = U_0^{(a)} \oplus U_1^{(a)}$, $U_0^{(a/4)} = U_0^{(a/2)} \oplus U_1^{(a/2)}$ etc. Therefore $U_0^{(2^l a)} = \sum_{m=l+1}^{\infty} \oplus U_1^{(2^m a)}$. When $l \to -\infty$, $U_0^{(2^l a)}$ reduces to $L^2(\mathbb{R})$. we can prove this fact by considering the Fourier transform

$$\int_{-\infty}^{\infty} \phi_0^{(2^l a)}(x - 2^l am) \mathrm{e}^{-\mathrm{i}kx'} \, \mathrm{d}x' = \widehat{\phi}_0^{(2^l a)}(k) \mathrm{e}^{-\mathrm{i}k2^l am} . \tag{3.18}$$

In the limit of $l \to -\infty$ keeping $2^l am \to x$, the right-hand side is nothing but $\mathrm{e}^{-\mathrm{i}kx}$ since the support of $\widehat{\phi}_0^{(2^l a)}(k)$ becomes infinitely large. Consequently $\lim_{l \to -\infty} U_0^{(2^l a)}$ reduces to the space spanned by $\{e^{ikx}; k, x \in \mathbb{R}\}$, i.e. $L^2(\mathbb{R})$. Considering the limit $l \to \infty$ in (3.18), we notice that

$$\bigcap_{l \in \mathbb{Z}s} U_0^{(2^l a)} = \{0\} \tag{3.19}$$

since the support of $\widehat{\phi}_0^{(2^l a)}(k)$ vanishes in this limit. From the above considerations, $L^2(\mathbb{R})$ can be decomposed into a sum of the orthogonal subspaces $U_1^{(2^l a)}$, $l \in \mathbb{Z}$:

$$L^2(\mathbb{R}) = \cdots \oplus U_1^{(2^1 a)} \oplus U_1^{(2^0 a)} \oplus U_1^{(2^{-1} a)} \oplus \cdots . \tag{3.20}$$

Using the relations (3.6) and (3.7), we can summarize the results shown above in the well known form in the multi-resolution analysis as follows:

$$L^2(\mathbb{R}) = \mathrm{clos}_{L^2(\mathbb{R})}\langle 2^{l/2}\phi_1^{(a)}(2^l \cdot -m) : m \in \mathbb{Z},\ l \in \mathbb{Z}\rangle \tag{3.21a}$$

$$\langle 2^{l_1/2}\phi_1^{(a)}(2^{l_1} \cdot -am_1), 2^{l_2/2}\phi_1^{(a)}(2^{l_2} \cdot -am_2)\rangle = \delta_{l_1,l_2}\delta_{m_1,m_2} \qquad l_1, l_2, m_1, m_2 \in \mathbb{Z}\,. \tag{3.21b}$$

We note that these properties of the Hilbert space or basis functions are the same as those for the wavelet analysis. In fact, the Wannier function $\phi_0^{(a)}$ of the zeroth band for a free electron is the scaling function or the father wavelet which generates a multi-resolution analysis, $\{U_0^{(2^l a)}\}$, $l \in \mathbb{Z}$, of $L^2(\mathbb{R})$. It is also called a sampling function in information theory. The Wannier function $\phi_1^{(a)}$ of a free electron of the first band is a kind of the orthogonal wavelets which generates the complementary subspaces, $\{U_1^{(2^l a)} : l \in \mathbb{Z}\}$, of the multi-resolution analysis and is known as Littlewood–Paley's mother wavelet [2]. In addition, the relation (3.6) and the decomposition property (A.3) in appendix A indicates that the Wannier functions $\phi_n^{(a)}$ for $n \geqslant 2$ are the wavelet packets [2, 3], and they are generated by the scaling function $\phi_0^{(a)}$ and the wavelet $\phi_1^{(a)}$ using the relations (A.7) and (A.8) in appendix A where we put

$$\begin{aligned} r_{m_1-2m_2}^{(n')\,*} &= \begin{cases} p_{m_1-2m_2} & \text{for} \quad n' = 2n \\ q_{m_1-2m_2} & \text{for} \quad n' = 2n+1 \\ 0 & \text{otherwise} \end{cases} \\ s_{m_1-2m_2}^{(n')\,*} &= \begin{cases} p_{m_1-2m_2} & \text{for} \quad n' = 2n+1 \\ q_{m_1-2m_2} & \text{for} \quad n' = 2n \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \tag{3.22}$$

4. Two-scale relations in general one-dimensional crystals

In this section, we consider the two-scale relations in general one-dimensional crystals. When the potential energy does not vanish, we cannot follow the procedure in section 3 which relies on the fact that the potential energy is identically zero. We first note that each Brillouin zone of a lattice with lattice constant a is enclosed by Bragg planes which are the bisector of a line joining the origin of k-space to a reciprocal lattice point $2\pi n/a$ for each $n \in \mathbb{Z}$. When we regard the crystal as that of lattice constant $2a$, new reciprocal lattice points $\{\pi(2n+1)/a\}$ appear, which generate corresponding Bragg planes, hence the Brillouin zones are decomposed into smaller ones (figure 1). Therefore the energy band $\varepsilon_n^{(a)}(k)$, $\pi n/a \leqslant |k| < \pi(n+1)/a$, of the nth Bloch state are composed of the energy band $\varepsilon_{2n}^{(2a)}(k)$, $\pi n/a \leqslant |k| < \pi(2n+1)/2a$, of the $2n$th Bloch state and

$\varepsilon_{2n+1}^{(2a)}$, $\pi(2n+1)/2a \leqslant |k| < \pi(n+1)/a$, of the $(2n+1)$th Bloch state for the same system with the renormalized lattice constant $2a$. Namely, we find

$$\varepsilon_n^{(a)}(k) = \begin{cases} \varepsilon_{2n}^{(2a)}(k) & \text{for} \quad \dfrac{\pi}{a}n \leqslant |k| < \dfrac{\pi}{2a}(2n+1) \\ \varepsilon_{2n+1}^{(2a)}(k) & \text{for} \quad \dfrac{\pi}{2a}(2n+1) \leqslant |k| < \dfrac{\pi}{a}(n+1) \,. \end{cases} \tag{4.1}$$

From the relation (A.4) in appendix A, we find that the relation between the Bloch functions for a lattice of lattice constant a and that for a lattice of renormalized lattice constant $2a$ is given by

$$\sqrt{2}\psi_{n,k}^{(a)}(x) = R_n^{(a)}(k)\psi_{2n,k}^{(2a)}(x) + S_n^{(a)}(k)\psi_{2n+1,k}^{(2a)}(x) \tag{4.2}$$

where the Bloch functions for lattice constant a, $\{\psi_{n,k}^{(a)}\}$, satisfy the normalization (2.3). To obtain the concrete form of the coefficients $R_n^{(a)}(k)$ and $S_n^{(a)}(k)$, we operate the Hamiltonian $H(x; a)$, possessing $\{\psi_{n,k}^{(a)}\}$ and $\{\psi_{n',k'}^{(2a)}\}$ as its eigenfunctions, to both sides of (4.2), where $H(x; a) = H(x; 2a)$. From the relation (4.1), we find

$$\varepsilon_n^{(a)}(k)\sqrt{2}\psi_{n,k}^{(a)}(x) = R_n^{(a)}(k)\varepsilon_{2n}^{(2a)}(k)\psi_{2n,k}^{(2a)}(x) + S_n^{(a)}(k)\varepsilon_{2n+1}^{(2a)}(k)\psi_{2n+1,k}^{(2a)}(x)\,. \tag{4.3}$$

Equations (4.1) and (4.3) give immediately the only possible form of $R_n^{(a)}(k)$ and $S_n^{(a)}(k)$

$$R_{2n}^{(a)}(k) = S_{2n+1}^{(a)} = P_a(k) \tag{4.4}$$

$$R_{2n+1}^{(a)}(k) = S_{2n}^{(a)} = Q_a(k) \tag{4.5}$$

for all $n \in \mathbb{Z}_+$, where $P_a(k)$ and $Q_a(k)$ are rectangular pulses with period $2\pi/a$ which are shown in figure 5. As a result, we obtain the decomposition relation of Bloch functions;

$$\sqrt{2}\psi_{2n,k}^{(a)}(x) = P_a^*(k)\psi_{4n,k}^{(2a)}(x) + Q_a^*(k)\psi_{4n+1,k}^{(2a)}(x) \tag{4.6a}$$

$$\sqrt{2}\psi_{2n+1,k}^{(a)}(x) = P_a^*(k)\psi_{4n+3,k}^{(2a)}(x) + Q_a^*(k)\psi_{4n+2,k}^{(2a)}(x)\,. \tag{4.6b}$$

Although $P_a(k)$ and $Q_a(k)$ are real in (4.6*a*) and (4.6*b*) we used their complex conjugates for later convenience.

We now proceed to the Wannier function representation of the decomposition relations (4.6*a*) and (4.6*b*). The decomposition relations of the Bloch function obtained above directly lead to that of the Wannier function. By the use of (2.4), equation (4.6*a*) reduces to

$$\sum_{m_1=-\infty}^{\infty} \phi_{2n}^{(a)}(x - am_1)\mathrm{e}^{\mathrm{i}kam_1} = P_a^*(k) \sum_{m_2=-\infty}^{\infty} \phi_{4n}^{(2a)}(x - 2am_2)\mathrm{e}^{\mathrm{i}k2am_2}$$
$$+ Q_a^*(k) \sum_{m_2=-\infty}^{\infty} \phi_{4n+1}^{(2a)}(x - 2am_2)\mathrm{e}^{\mathrm{i}k2am_2}\,. \tag{4.7}$$

Since $P_a^*(k)$ and $Q_a^*(k)$ are $2\pi/a$-periodic functions, they can be expanded in Fourier series representations

$$P_a^*(k) = \sum_{m=-\infty}^{\infty} p_m^* \mathrm{e}^{\mathrm{i}kam} \tag{4.8a}$$

$$Q_a^*(k) = \sum_{m=-\infty}^{\infty} q_m^* \mathrm{e}^{\mathrm{i}kam}\,. \tag{4.8b}$$

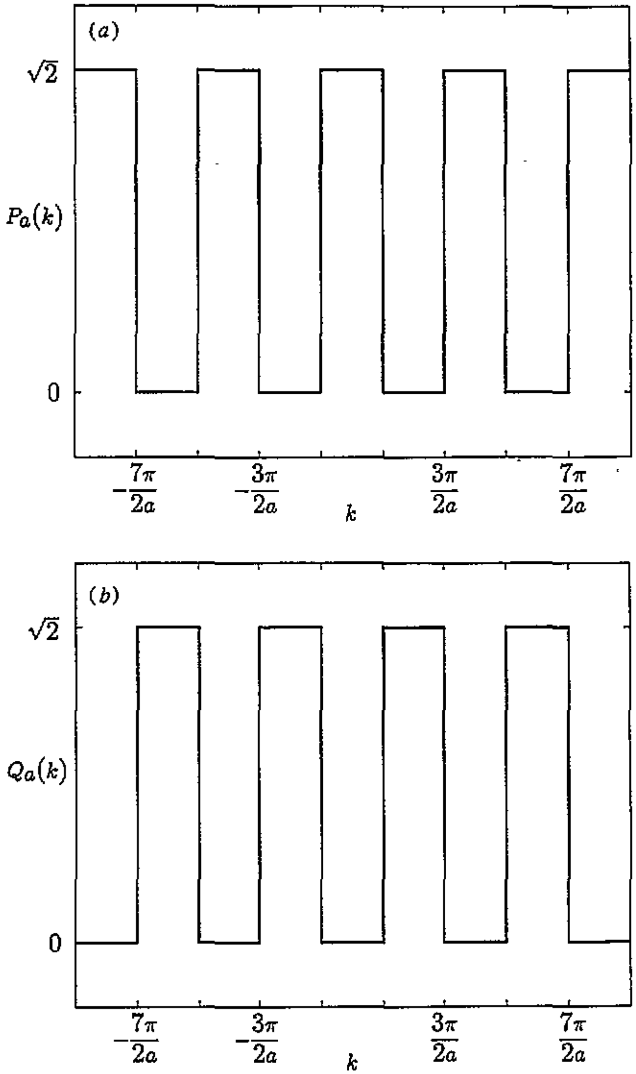

Figure 5. The k dependence of (a) $P_a(k)$ and (b) $Q_a(k)$, which are periodic functions of period $2\pi/a$.

Here the coefficients $\{p_m\}$ and $\{q_m\}$ are given by (3.9a) and (3.9b), and they do not depend on lattice constant a. Using equations (4.8a) and (4.8b), equation (4.7) is rewritten as

$$\phi_{2n}^{(a)}(x - am_1) = \sum_{m_2=-\infty}^{\infty} p_{m_1-2m_2}^{*} \phi_{4n}^{(2a)}(x - 2am_2) + \sum_{m_2=-\infty}^{\infty} q_{m_1-2m_2}^{*} \phi_{4n+1}^{(2a)}(x - 2am_2) . \tag{4.9a}$$

Applying the same procedure to (4.6b), we find

$$\phi_{2n+1}^{(a)}(x - am_1) = \sum_{m_2=-\infty}^{\infty} p_{m_1-2m_2}^{*} \phi_{4n+3}^{(2a)}(x - 2am_2) + \sum_{m_2=-\infty}^{\infty} q_{m_1-2m_2}^{*} \phi_{4n+2}^{(2a)}(x - 2am_2) . \tag{4.9b}$$

The relations (4.9*a*) and (4.9*b*) are the decomposition relations of the Wannier functions for general one-dimensional lattices.

It is straightforward to derive the two-scale relations corresponding to (3.10*a*)–(3.10*d*). We first note that both Wannier functions $\phi_{2n}^{(2a)}(\in U_{2n}^{(2a)})$ and $\phi_{2n+1}^{(2a)}(\in U_{2n+1}^{(2a)})$ of the lattice with the inflated lattice constant $2a$ belong to $U_n^{(a)}$ (see equation (A.4) in appendix A). Therefore, noting $U_n^{(a)}$ is generated by the linear span of $\phi_n^{(a)}(x-ma),\ m \in \mathbb{Z}$, we find the following two-scale relations of Wannier functions

$$\phi_{4n}^{(2a)}(x) = \sum_{m=-\infty}^{\infty} p_m \phi_{2n}^{(a)}(x-am) \tag{4.10a}$$

$$\phi_{4n+1}^{(2a)}(x) = \sum_{m=-\infty}^{\infty} q_m \phi_{2n}^{(a)}(x-am) \tag{4.10b}$$

$$\phi_{4n+3}^{(2a)}(x) = \sum_{m=-\infty}^{\infty} p_m \phi_{2n+1}^{(a)}(x-am) \tag{4.10c}$$

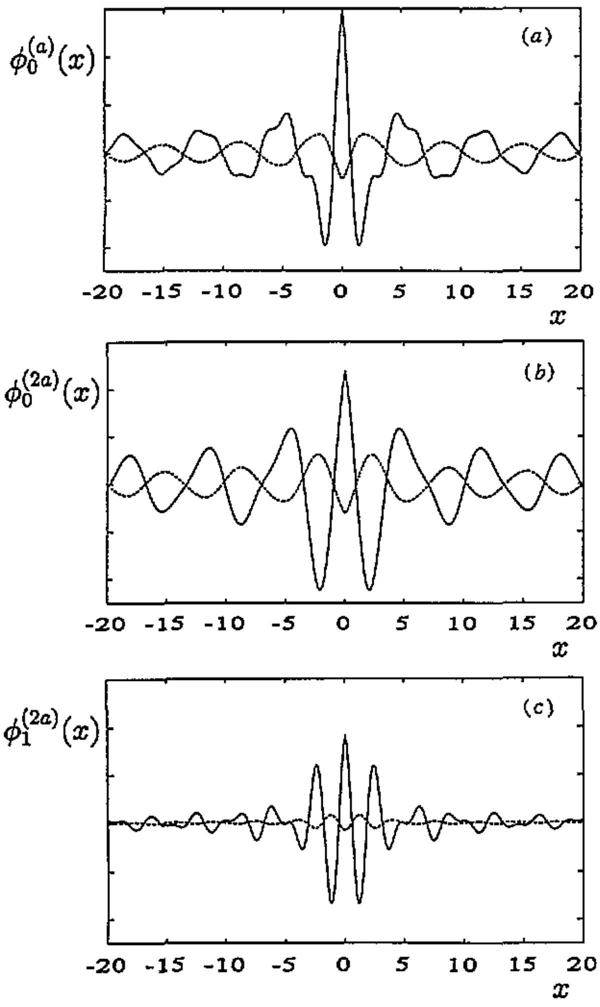

Figure 6. (*a*) Wannier function around the origin in the lowest band for the Kronig–Penney model. (*b*) Wannier function around the origin in the lowest band for the Kronig–Penney model when the lattice constant is taken as $2a$. (*c*) Wannier function around the origin in the first excited band for the Kronig–Penney model when the lattice constant is taken as $2a$. The real parts are denoted by full curves, and the imaginary parts are denoted by broken curves.

$$\phi_{4n+2}^{(2a)}(x) = \sum_{m=-\infty}^{\infty} q_m \phi_{2n+1}^{(a)}(x - am). \tag{4.10d}$$

The form of the decomposition relations (4.9*a*) and (4.9*b*) and the two-scale relations (4.10*a*)–(4.10*d*) are the same as equations (A.5), (A.7) and (A.8) in appendix A where the coefficients $\{r_m^{(n)}\}$ and $\{s_m^{(n)}\}$ are given by (3.22) with the coefficients $\{p_m\}$ and $\{q_m\}$ given in (3.9*a*) and (3.9*b*).

It should be emphasized that although (4.9*a*), (4.9*b*) and (4.10*a*)–(4.10*d*) are similar to the two-scale relations (3.10*a*)–(3.10*d*) for a free electron, there is a significant difference between them. This difference originates from the relation (3.6) which is only valid for the Wannier functions for a free electron. Equations (3.10*a*)–(3.10*d*) and (3.11*a*), (3.11*b*) are relations among the Wannier functions of the same lattice constant a and differently scaled x-coordinate. On the other hand, equations (4.9*a*), (4.9*b*) and (4.10*a*)–(4.10*d*) are relations among the Wannier functions of the different lattice constants and the same scale of x-coordinate. In particular, when $n = 0$ the Wannier functions of (3.10*a*) have the same form which leads to the two-scale relation of the scaling function in the wavelet analysis. However, the Wannier functions in (4.10*a*) for $n = 0$, $\phi_0^{(2a)}(x)$ and $\phi_0^{(a)}(x)$, are not the same function. Hence the Wannier functions of a system with finite potential are not the wavelet packets. Nevertheless, we can state that the Wannier functions for a lattice constant $2a$ are generated by the Wannier functions of the same system with lattice constant a using the same linear combinations as those which generate the wavelet packets.

As an example, we consider the Kronig–Penney model

$$H = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{m=-\infty}^{\infty} g\delta(x - ma). \tag{4.11}$$

To construct the concrete form of the Wannier function, we follow the standard procedure to obtain the energy bands and Bloch functions [1], which is summarized in appendix B. Figure 6(*a*) shows the Wannier function $\phi_0^{(a)}(x)$ in the lowest band, where we solved (B.6) numerically setting $\hbar^2/2M = g = a = 1.0$. To obtain this Wannier function, we set the k-dependent arbitrary phase factor in the Bloch function so that $A(K, k)$ in appendix B becomes real. In figures 6(*b*) and (*c*) we show the lower most two bands of the Wannier functions $\phi_0^{(2a)}(x)$ and $\phi_1^{(2a)}(x)$ for the two fold scaled system. They are obtained using the relation (2.5) imposing $a \to 2a$ and related to $\phi_0^{(a)}(x - am)$ by (4.9*a*), (4.10*a*) and (4.10*b*) for $n = 0$. As can be seen, two differently scaled Wannier functions $\phi_0^{(a)}$ and $\phi_0^{(2a)}$ have a different form to each other, namely, they are not the wavelet packets.

5. Translational symmetry and two-scale relation

When one takes a larger cell as the periodic unit of the translational symmetry, some operations in the translational symmetry must be discarded. It is, however, clear that the energy bands and the Bloch functions should not depend on the choice of the periodic unit (see equations (4.6*a*) and (4.6*b*)). This fact indicates that the Wannier functions based on a larger unit cell must be influenced by translational symmetry operations. To emphasize this point, we consider a model system of an electron in one dimension whose Hamiltonian is given by

$$H = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{m=-\infty}^{\infty} v(x - ma) \tag{5.1}$$

where

$$v(x) = \begin{cases} V & V \longrightarrow \infty \quad \text{for } -\frac{b}{2} \leqslant x \leqslant \frac{b}{2} \\ 0 & \text{otherwise} \end{cases} \tag{5.2}$$

for $a > b > 0$. Namely, potential wells of zero potential with width $a - b$ are placed periodically with period a, which are separated by infinitely high potential-barriers with width b. We follow the procedure in appendix B. For the potential energy (5.2), we can set

$$t_+ = t_- = 0 \qquad r_+ = r_- = -e^{-iKb} \tag{5.3}$$

in equation (B.6), where K is the wavenumber of the incident particle. Then, from equation (B.3) and the normalization condition (2.3), we obtain the energy band and the Bloch function

$$\varepsilon_{n,k}^{(a)} = \varepsilon_n^{(a)} = \frac{\hbar^2 n^2 \pi^2}{2M(a-b)^2} \tag{5.4}$$

$$\begin{aligned} \psi_{K,k}^{(a)}(x) &= \psi_{n,k}^{(a)}(x) \\ &= \sum_{m=-\infty}^{\infty} \sqrt{\frac{a}{\pi(a-b)}} \sin\left\{\frac{\pi}{a-b} n\left(x - \frac{b}{2} - am\right)\right\} e^{ikam} \chi_{[ma,(m+1)a]}(x) \end{aligned} \tag{5.5}$$

for $n \in \mathbb{Z}_+$ and the characteristic function $\chi_{[\alpha,\beta]}(x)$ is unity in the range $\alpha + b/2 \leqslant x \leqslant \beta - b/2$ and zero otherwise. The prefactor $\sqrt{a/\pi(a-b)}$ assures the normalization condition (2.3). As can be seen in (4.6a) and (4.6b), this Bloch function should not depend on whether we view the lattice constant to be a or $2a$, if we choose the appropriate Brillouin zones and the band index n; namely,

$$\psi_{2n,k}^{(2a)} = \psi_{n,k}^{(a)} \qquad \text{for} \quad \frac{\pi}{2a} 2n \leqslant |k| < \frac{\pi}{2a}(2n+1) \tag{5.6a}$$

$$\psi_{2n+1,k}^{(2a)} = \psi_{n,k}^{(a)} \qquad \text{for} \quad \frac{\pi}{2a}(2n+1) \leqslant |k| < \frac{\pi}{2a}(2n+2)\,. \tag{5.6b}$$

The Wannier function is readily obtained from (2.5) and (5.5) as

$$\phi_n^{(a)}(x - am) = \sqrt{\frac{2}{a-b}} \sin\left\{\frac{\pi}{a-b} n\left(x - \frac{b}{2} - am\right)\right\} \chi_{[ma,(m+1)a]}(x) \tag{5.7}$$

for $m \in \mathbb{Z}$. Note that this Wannier functions is nothing but a state in one potential well.

Now we insert (5.6a) and (5.6b) into (2.5) (where we put $a \to 2a$) to obtain the renormalized Wannier functions (with lattice constant $2a$) such as

$$\begin{aligned} \phi_{2n}^{(2a)}(x - 2am') &= \sqrt{\frac{2a}{2\pi}} \int_{-\frac{\pi}{2a}(2n+1)}^{-\frac{\pi}{2a}2n} dk\, \psi_{2n,k}^{(2a)}(x) e^{-ika2m'} + \sqrt{\frac{2a}{2\pi}} \int_{\frac{\pi}{2a}2n}^{\frac{\pi}{2a}(2n+1)} dk\, \psi_{2n,k}^{(2a)}(x) e^{-ika2m'} \\ &= \sum_{m(\neq 2m')} \frac{\sqrt{2}\sin\{\pi(2n+1)(m-2m')/2\}}{\pi(m-2m')} \phi_n^{(a)}(x - am) \\ &\quad + \frac{1}{\sqrt{2}} \phi_n^{(a)}(x - 2am') \end{aligned} \tag{5.8a}$$

$$\begin{aligned} \phi_{2n+1}^{(2a)}(x - 2am') &= \sqrt{\frac{2a}{2\pi}} \int_{-\frac{\pi}{2a}(2n+2)}^{-\frac{\pi}{2a}(2n+1)} dk\, \psi_{2n+1,k}^{(2a)}(x) e^{-ika2m'} \\ &\quad + \sqrt{\frac{2a}{2\pi}} \int_{\frac{\pi}{2a}(2n+1)}^{\frac{\pi}{2a}(2n+2)} dk\, \psi_{2n+1,k}^{(2a)}(x) e^{-ika2m'} \end{aligned}$$

$$= -\sum_{m(\neq 2m')} \frac{\sqrt{2}\sin\{\pi(2n+1)(m-2m')/2\}}{\pi(m-2m')}\phi_n^{(a)}(x-am) + \frac{1}{\sqrt{2}}\phi_n^{(a)}(x-2am'). \tag{5.8b}$$

Notice that although these expressions are a superposition of $\phi_n^{(a)}(x-am)$, only one term on the right-hand side does not vanish for a given value of x because of (5.7). Since

$$\begin{aligned} \frac{\sqrt{2}\sin\{\pi(2n'+1)(m_1-2m_2)/2\}}{\pi(m_1-2m_2)} &= \begin{cases} p_{m_1-2m_2} & \text{for} \quad n'=2n \\ q_{m_1-2m_2} & \text{for} \quad n'=2n+1 \end{cases} \\ -\frac{\sqrt{2}\sin\{\pi(2n'+1)(m_1-2m_2)/2\}}{\pi(m_1-2m_2)} &= \begin{cases} p_{m_1-2m_2} & \text{for} \quad n'=2n+1 \\ q_{m_1-2m_2} & \text{for} \quad n'=2n \end{cases} \end{aligned} \tag{5.9}$$

for $n \in \mathbb{Z}_+$, $m_1 \neq 2m_2$ and $p_0 = 1/\sqrt{2}$ and $q_0 = 1/\sqrt{2}$, equations (5.8a) and (5.8b) are consistent with the two-scale relation (4.10a)–(4.10d). Hence it should be emphasized that these weight factors $\{p_m\}$ and $\{q_m\}$ for a superposition are the consequence of the missing translational symmetry in the inflated lattice.

Suppose we take two adjacent potential wells as a periodic unit and make the lattice constant to be $2a$. Since there is an infinite potential barrier between these periodic units, we may consider the localized Wannier functions in a periodic unit with width $2a$ to be Wannier functions which are given by

$$\begin{aligned} \phi'^{(2a)}_{2n}(x-2m'a) = \frac{1}{\sqrt{2}}\Bigg\{&\sqrt{\frac{2}{a-b}}\sin\left[\frac{\pi}{a-b}n\left(x-\frac{b}{2}-2m'a\right)\right]\chi_{[2m'a,(2m'+1)a]}(x) \\ &+\sqrt{\frac{2}{a-b}}\sin\left[\frac{\pi}{a-b}n\left(x-\frac{b}{2}-(2m'+1)a\right)\right]\chi_{[(2m'+1)a,2(m'+1)a]}(x)\Bigg\} \end{aligned} \tag{5.10a}$$

$$\begin{aligned} \phi'^{(2a)}_{2n+1}(x-2m'a) = \frac{1}{\sqrt{2}}\Bigg\{&\sqrt{\frac{2}{a-b}}\sin\left[\frac{\pi}{a-b}n\left(x-\frac{b}{2}-2m'a\right)\right]\chi_{[2m'a,(2m'+1)a]}(x) \\ &-\sqrt{\frac{2}{a-b}}\sin\left[\frac{\pi}{a-b}n\left(x-\frac{b}{2}-(2m'+1)a\right)\right]\chi_{[(2m'+1)a,2(m'+1)a]}(x)\Bigg\} \end{aligned} \tag{5.10b}$$

for all $m' \in \mathbb{Z}$, $n \in \mathbb{Z}_+$. The two degenerated Wannier states (5.10a) and (5.10b) are the eigenstates of the system composed of only two potential wells located on $x = 2m'a$ and $x = (2m'+1)a$ with the energy $(\hbar\pi n)^2/2Ma^2$. Namely $\phi'^{(2a)}_{2n}(x)$ is even with respect to the inversion operation, and $\phi'^{(2a)}_{2n+1}(x)$ is odd. Using equations (5.10a), (5.10b) and (2.4), we obtain the Bloch functions for a lattice with the minimal lattice constant is $2a$

$$\begin{aligned} \psi'^{(2a)}_{2n,k}(x) = \sqrt{\frac{a}{\pi(a-b)}}\Bigg\{&\sin\left[\frac{\pi}{a-b}n\left(x-\frac{b}{2}-2ma\right)\right]\chi_{[2m'a,(2m'+1)a]}(x) \\ &+\sin\left[\frac{\pi}{a}n\left(x-\frac{b}{2}-(2m+1)a\right)\right]\chi_{[(2m'+1)a,2(m'+1)a]}(x)\Bigg\}\,\mathrm{e}^{ika2m} \\ &\text{for} \quad 2ma < x < 2(m+1)a. \end{aligned} \tag{5.11}$$

The difference between the Bloch functions (5.5) and (5.11) is evident. Namely, the inversion symmetry of $\phi'^{(2a)}_{2n}$ and $\phi'^{(2a)}_{2n+1}$ in (5.10a) and (5.10b) is consistent with the translational symmetry with lattice constant $2a$, but is not consistent with the translational symmetry with lattice constant a. Hence, equation (5.11) is not the eigenfunction of the Hamiltonian (5.1). This paradox is due to the fact that some part of the translational symmetry is missing in the lattice which is assumed to have a larger lattice constant.

6. Summary

We have presented a complete analysis of the Bloch functions and the Wannier functions in one dimension when the size of the periodic unit is taken as twice as large as the primitive cell. The two-scale coefficients $\{p_m\}$ and $\{q_m\}$ or the $2\pi/a$-periodic functions $P_a(k)$ and $Q_a(k)$ which have $\{p_m\}$ and $\{q_m\}$ as their Fourier series representations give the invariant means for the renormalization transformation in one-dimensional periodic systems. If the periodic potential energy is finite, then the Wannier functions of the system change their forms when one takes a larger unit cell. However, the two-scale coefficients remains invariant and they do not depend on the form of the potential energy. It is known that although the energy band is folded into smaller Brillouin zone when the lattice constant is renormalized, the reciprocal lattice does not change effectively because of the structure factor. This property of the energy band is related to the fact that the two-scale coefficients do not depend on the potential energy.

The Wannier functions for a free electron do not change their representations through such a renormalization procedure. In other words the Wannier function for a free electron plays the role of a generating function of such two-scale coefficients, and they are shown to have the properties of wavelet analysis. Some properties seen in the Wannier functions of the first excited band for a free electron are those of the orthogonal wavelets itself, and the free electron Wannier functions of the higher excited levels are generated from the zeroth and first band's Wannier functions using the two-scale coefficients $\{p_m\}$ and $\{q_m\}$, and this algorithm is nothing but the way that the wavelet packets are generated in the multi-resolution analysis.

Appendix A. Two-scale relation of the subspaces in $L^2(\mathbb{R})$

We consider the eigenstates of one electron in a general one-dimensional lattice. The following arguement does not assume any particular form to the potential energy.

For each band index n, let $U_n^{(a)}$ denote the linear span of Wannier functions $\{\phi_n^{(a)}(\cdot - am) : m \in \mathbb{Z}\}$, namely,

$$U_n^{(a)} = \mathrm{clos}_{L^2(\mathbb{R})}\langle\phi_n^{(a)}(\cdot - am) : m \in \mathbb{Z}\rangle \qquad n \in \mathbb{Z}_+ \tag{A.1}$$

where the sign '$\mathrm{clos}_{L^2(\mathbb{R})}$' denotes the closure of $L^2(\mathbb{R})$ space. In the following, we argue the decomposition property of $L^2(\mathbb{R})$ by the subspace $U_n^{(a)}$. Obviously $U_n^{(a)}$ can also be considered as the subspace of $L^2(\mathbb{R})$ spanned by the set of the Bloch functions $\{\psi_{n,k}^{(a)}(\cdot) : \pi n/a \leqslant |k| < \pi(n+1)/a\}$, namely,

$$U_n^{(a)} = \mathrm{clos}_{L^2(\mathbb{R})}\langle\psi_{n,k}^{(a)}(\cdot) : \frac{\pi}{a}n \leqslant |k| < \frac{\pi}{a}(n+1)\rangle. \tag{A.2}$$

From the well known orthonormality of the Bloch functions, $U_n^{(a)}$ for $n \in \mathbb{Z}_+$ form orthogonal summands of $L^2(\mathbb{R})$, namely

$$L^2(\mathbb{R}) = U_0^{(a)} \oplus U_1^{(a)} \oplus U_2^{(a)} \oplus \cdots. \tag{A.3}$$

It is clear that the Brillouin zone for the $2n$th and $(2n+1)$th bands of Bloch states with period $2a$ are $\pi 2n/2a \leqslant |k| < \pi(2n+1)/2a$ and $\pi(2n+1)/2a \leqslant |k| < \pi(2n+2)/2a$, respectively. These supports in k space are complements of the support of the nth band of Bloch states with period a. Therefore the spaces $U_{2n}^{(2a)}$ and $U_{2n+1}^{(2a)}$ are orthogonal summands of $U_n^{(a)}$, i.e. $U_n^{(a)}$ is decomposed as

$$U_n^{(a)} = U_{2n}^{(2a)} \oplus U_{2n+1}^{(2a)} . \tag{A.4}$$

Hence, immediately we find the following decomposition relations of the Wannier functions:

$$\phi_n^{(a)}(x - am_1) = \sum_{m_2=-\infty}^{\infty} r_{m_1-2m_2}^{(n)} \phi_{2n}^{(2a)}(x - 2am_2) + \sum_{m_2=-\infty}^{\infty} s_{m_1-2m_2}^{(n)} \phi_{2n+1}^{(2a)}(x - 2am_2) \tag{A.5}$$

for all $m_1 \in \mathbb{Z}$, where the coefficients $\{r_m^{(n)}\}$ and $\{s_m^{(n)}\}$ are defined as the inner products of the Wannier functions of different lattice constant:

$$\langle \phi_{n'}^{(2a)}(\cdot - 2am_1), \phi_n^{(a)}(\cdot - am_2)\rangle = \begin{cases} r_{m_1-2m_2}^{(n)} & \text{for} \quad n' = 2n \\ s_{m_1-2m_2}^{(n)} & \text{for} \quad n' = 2n+1 \\ 0 & \text{otherwise} . \end{cases} \tag{A.6}$$

The inverse transformations of the decomposition relations (A.5) are the two-scale relations:

$$\phi_{2n}^{(2a)}(x - 2am_2) = \sum_{m_1=-\infty}^{\infty} r_{m_1-2m_2}^{(n)\,*} \phi_n^{(a)}(x - am_1) \tag{A.7}$$

$$\phi_{2n+1}^{(2a)}(x - 2am_2) = \sum_{m_1=-\infty}^{\infty} s_{m_1-2m_2}^{(n)\,*} \phi_n^{(a)}(x - am_1) . \tag{A.8}$$

From the direct calculations of the inner product of the Wannier functions (A.5), (A.7) and (A.8), we obtain the following orthogonality relations:

$$\sum_{m=-\infty}^{\infty} r_{m-2m_1}^{(n)} r_{m-2m_2}^{(n)\,*} = \delta_{m_1,m_2} \tag{A.9}$$

$$\sum_{m=-\infty}^{\infty} s_{m-2m_1}^{(n)} s_{m-2m_2}^{(n)\,*} = \delta_{m_1,m_2} \tag{A.10}$$

$$\sum_{m=-\infty}^{\infty} r_{m-2m_1}^{(n)} s_{m-2m_2}^{(n)\,*} = 0 \tag{A.11}$$

$$\sum_{m=-\infty}^{\infty} \left\{ r_{m_1-2m}^{(n)} r_{m_2-2m}^{(n)\,*} + s_{m_1-2m}^{(n)} s_{m_2-2m}^{(n)\,*} \right\} = \delta_{m_1,m_2} \tag{A.12}$$

for all $m_1, m_2 \in \mathbb{Z}$. These relations for the coefficients $\{r_m^{(n)}\}$ and $\{s_m^{(n)}\}$ are the basis of the two-scale transformations between the basis functions of the subspaces $U_{2n}^{(2a)}$, $U_{2n+1}^{(2a)}$ and $U_n^{(a)}$. These coefficients becomes the two-scale coefficients of the wavelet analysis when they have the special n-dependence (3.22). In this case the orthogonality relations (A.9)–(A.12) allow the coefficients $\{r_m^{(n)}\}$ and $\{s_m^{(n)}\}$ to generate wavelets and wavelet packets.

Appendix B. Single potential-barrier problem and Bloch states

In one-dimensional periodic systems the band structure and the Bloch functions can be determined by the properties of an electron in a single potential barrier $v(x)$ [1]. We set the support of $v(x)$; $-b/2 \leqslant x \leqslant b/2$, where b is smaller than the period, $-a/2 \leqslant x \leqslant a/2$, of the system. Let $t_+(K)$ and $r_+(K)$ be the transmission and reflection coefficients of a particle with the energy $\hbar^2K^2/2M$ incident from the left ($x < 0$) on the single potential-barrier. Then in the region $|x| > b/2$, the steady-state wavefunction $\psi_l(x)$ have the form

$$\begin{aligned}\psi_l(x) &= e^{iKx} + r_+(K)e^{-iKx} \qquad x < -b/2 \\ &= t_+(K)e^{iKx} \qquad x > b/2 .\end{aligned} \tag{B.1}$$

Similarly, the wavefunction of a particle incident from the right ($x > 0$) has the form

$$\begin{aligned}\psi_r(x) &= t_-(K)e^{-iKx} \qquad x < -b/2 \\ &= e^{-iKx} + r_-(K)e^{iKx} \qquad x > b/2\end{aligned} \tag{B.2}$$

where $t_-(K)$ and $r_-(K)$ are the transmission and reflection coefficients of a particle with the energy $\hbar^2K^2/2M$ incident from the right on a single barrier. Now the Bloch function with crystal momentum k can be expressed as the superposition of ψ_l and ψ_r:

$$\psi^{(a)}_{K,k}(x) = A(K,k)\psi_l(x) + B(K,k)\psi_r(x) \qquad b/2 < |x| \leqslant a/2 . \tag{B.3}$$

The substitution of the Bloch conditions

$$\psi_{K,k}(x+a)\big|_{x=-a/2} = e^{ika}\psi_{K,k}(x)\big|_{x=-a/2} \tag{B.4}$$

$$\frac{d}{dx}\psi_{K,k}(x+a)\bigg|_{x=-a/2} = e^{ika}\frac{d}{dx}\psi_{K,k}(x)\bigg|_{x=-a/2} \tag{B.5}$$

to equation (B.3) leads to the relations between K and crystal momentum k:

$$\begin{pmatrix} t_+(K) & r_-(K) \\ r_+(K) & t_-(K) \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = e^{-iKa}\begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} . \tag{B.6}$$

From the knowledge of $t_\pm(K)$ and $r_\pm(K)$ we can determine the relation between K and k, from which we find the energy band, and the relation of $A(K,k)$ and $B(K,k)$. Using the equation (B.3) and normalization condition (2.3), we obtain the Bloch function in the region $b/2 < |x| \leqslant a/2$.

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References

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For the deduction of the one-dimensional energy band structure, especially in the case of Kronig–Penney model, see problem 1 of chapter 8. Chapter 10 is devoted to the descriptions for the Wannier functions.

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For the wavelet packets, see chapter 7.