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Wannier functions of elliptic one-gap potential

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Abstract

Wannier functions of the one-dimensional Schrödinger equation with an elliptic one-gap potential are explicitly constructed. Properties of these functions are analytically and numerically investigated. In particular, we derive an expression for the amplitude of the Wannier function in the origin, a power series expansion valid in the vicinity of the origin and an asymptotic expansion characterizing the decay of the Wannier function at large distances. Using these results, we construct an approximate analytical expression of the Wannier function, which is valid in the whole spatial domain and is in good agreement with numerical results.

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1. Introduction

The spectral analysis of Schrödinger operators with periodic potentials has been investigated since the foundation of quantum mechanics. In spite of this, it still represents a non-exhausted topic of continuing interest. On the one hand, it plays a crucial role in condensed matter physics, where it provides the mathematical basis for the quantum theory of solids. On the other, Schrödinger operators with periodic and quasi-periodic potentials play an important role in the integration of the Kortweg–de Vries (KdV) equation. Eigenstates of these operators, also called Bloch functions (BF), have been extensively studied over recent years by different authors (see [1–3]). An expression of BF in terms of hyperelliptic θ-functions was given in [4]. These studies were further developed in [5], where an algebro-geometric scheme for constructing the solutions of non-linear equations was given in terms of the Baker–Akhiezer function. This function is uniquely defined on the Riemann surface associated with the energy spectrum and its properties are natural generalizations of the analytical properties of the BF of finite-gap potentials.

Besides BF, another set of functions that play an equally important role in condensed matter physics are the Wannier functions (WF) [6]. These functions are related to BF by a unitary transformation and form a complete set of localized orthonormal functions spanning a Bloch band. The properties of these functions were first investigated by Kohn [7] in 1959 in a classical paper, in which the asymptotic decay of WF was characterized for the case of centro-symmetrical one-dimensional potentials. Since then, a number of studies have been devoted to this topic, but we mention here the results of only some of them. The projection operator technique was developed for the construction of WF which were studied in the n-dimensional lattices [8, 9]. The localization problem for the WF was considered in a one-dimensional case [10]. These functions were utilized with success in new practical methods for the calculation of the electron energy of solids (see e.g. [11]) and in a number of modern calculation problems such as photonic crystal circuits [12]. WF represent the ideal basis for constructing effective Hamiltonians of quantum problems involving the spatial localizations induced by electric and magnetic fields [13–16].

In spite of this, the properties of these functions are still not fully understood and, except for the simplest cases, there are no models for which the analytical expression of the WF can be explicitly given. On the other hand, recent results obtained in the field of completely integrable systems open the possibility of investigating the analytical properties of the WF. Quite interestingly, WF have not been considered in the field of finite-gap potentials so far.

The present paper represents the first contribution in this direction. In particular, we consider WF of Schrödinger operators with one-gap potentials and use the well-developed theory of elliptic functions to investigate their properties with sufficient completeness. As a result, we derive (i) an exact value for the amplitude of the WF at the localization site, (ii) an asymptotic expansion characterizing the decay of the WF at large distances and (iii) a power series expansion valid in the vicinity of the localization site. Using results (ii) and (iii), we construct an approximate analytical representation of the WF, which is valid in the whole spatial domain. These results are shown to be in very good agreement with the WF obtained by means of numerical methods.

This paper is organized as follows. In section 2, we discuss the basic properties of the BF for one-gap potentials. In particular, we introduce the basic definitions, discuss the basic properties of BF and derive the analytical expressions of their normalization constants. Section 3 is devoted to a study of the WF. After recalling the basic definitions, we derive the main results of the paper, namely points (i)–(iii) listed above. In section 4, we construct an approximate analytical expression of the WF and compare the results of our theory with WF obtained from the basic definition using numerical tools. Finally, in section 5, we summarize the main results of the paper and briefly discuss future developments.

2. Properties of the Bloch functions of one-gap potentials

2.1. The Schrödinger equation with one-gap potentials

In this paper, we use the standard notations and facts of the theory of elliptic functions. In particular, we use the well-known Weierstrass $\wp$-, σ- and ζ-functions. For the benefit of the reader unfamiliar with elliptic functions, we recall that the Weierstrass elliptic $\wp$-function, $\wp(u) \equiv \wp(u|2\omega, 2\omega')$, and ζ-function, $\zeta(u) \equiv \zeta(u|2\omega, 2\omega')$, depend on the complex variable $u \in \mathbb{C}$ and also on two periods, the real period 2ω and the pure imaginary period $2\omega'$. Both functions are expressed in terms of the σ-function as

$$\wp(u) = -\frac{\partial^2}{\partial u^2} \log \sigma(u), \qquad \zeta(u) = \frac{\partial}{\partial u} \log \sigma(u),$$

where the σ-function, in particular, can be defined as the infinite product

$$\sigma(u) = u \prod{}' \left\{ \left(1 - \frac{u}{w}\right) \exp\left[\frac{z}{w} + \frac{1}{2} \left(\frac{z}{w}\right)^2 \right] \right\},$$

where the apex on the product sign indicates that, in taking all the possible values of $w = 2n\omega + 2m\omega'$ with n, m integers, the combination $n = m = 0$ must be excluded. The Weierstrass $\wp$-function is even and double-periodic (elliptic):

$$\wp(u + 2\omega) = \wp(u + 2\omega') = \wp(\omega),$$

whereas the ζ-function admits the following periodicity properties:

$$\zeta(u + 2\omega) = \zeta(u) + 2\eta, \qquad \zeta(u + 2\omega') = \zeta(u) + 2\eta', \qquad \eta = \zeta(\omega), \qquad \eta' = \zeta(\omega').$$

In the following, we adopt the classical notation, according to which, except for ω' and η' (where the prime denotes the imaginary half-period and the value of the ζ-function at the imaginary half-period, respectively), the 'prime' appearing in other letters will always denote the derivative with respect to the argument.

For our considerations, it is convenient to fix the following form of the potential:

$$\begin{aligned} &\mathcal{U}(x) = -2\wp(u), \qquad u = \mathrm{i}x + \omega, \quad x \in \mathbb{R}, \\ &\mathcal{U}(x + nT) = \mathcal{U}(x), \quad n \in \mathbb{N}, \end{aligned} \tag{2.1}$$

where $T = -2\mathrm{i}\omega'$ is the period of the lattice. Notice that T is real and $\mathcal{U}(x) = 2\wp(\mathrm{i}x + \omega)$ is a smooth periodic real function for all values of ω and ω'. Indeed,

$$\overline{\mathcal{U}(x)} = 2\wp(-\mathrm{i}x + \omega) = 2\wp(-\mathrm{i}x - \omega + 2\omega) = 2\wp(\mathrm{i}x + \omega) = \mathcal{U}(x),$$

where eveness and periodicity properties of the $\wp$-function were used.

The time-independent Schrödinger equation associated with the potential (2.1) is

$$\partial_x^2 \Psi(x; E) + (E - \mathcal{U}(x))\Psi(x; E) = 0. \tag{2.2}$$

As is well known (see e.g. [17] and references therein), this equation admits a spectrum that has a gap structure and eigenfunctions $\Psi(x; E)$ satisfying the Bloch condition

$$\Psi(x - T; E) = \mathrm{e}^{-\mathrm{i}k(E)T} \Psi(x; E), \tag{2.3}$$

where E is the energy given by

$$E = \wp(v), \qquad v = \alpha + \omega', \quad \alpha \in \mathbb{R}, \tag{2.4}$$

and $k(E)$ is the quasi-momentum given by

$$k(v) = \zeta(v) - \frac{\eta'}{\omega'} v, \qquad v = \alpha + \omega', \quad \alpha \in \mathbb{R}. \tag{2.5}$$

In the following, the half-periods ω and ω' will be considered as free parameters of the theory. Eigenfunctions of type (2.3) are called Bloch functions. Notice that the dependence of the quasi-momentum on energy (and vice versa) arises from elimination of the parameter α from equations (2.4) and (2.5). The BF can be written in explicit form as

$$\Psi(u; v) = C(v)\frac{\sigma(v-u)}{\sigma(v)\sigma(u)}\exp\{u\zeta(\alpha)\}, \tag{2.6}$$

or, alternatively, as

$$\Psi(u, v) = D(v)\sqrt{\wp(u)-\wp(v)}\,\exp\left\{\frac{\wp'(v)}{2}\int^{x}\frac{\mathrm{d}u}{\wp(u)-\wp(v)}\right\}, \tag{2.7}$$

where $C(v), D(v)$ are normalization constants that will be computed explicitly in terms of elliptic functions. In the following, we shall use both representations for the BF. Notice that the BF considered as a function of k is periodic in the reciprocal space with a period

$$2\widetilde{\omega} = \frac{\mathrm{i}\pi}{\omega'}.$$

BF has the following periodicity properties:

$$\Psi(u+2n\omega; v) = \exp\{2n\omega k(v)\}\Psi(u; v), \qquad k(v) = \zeta(v) - v\frac{\eta}{\omega}, \tag{2.8}$$

$$\Psi(u+2n'\omega'; v) = \exp\{2n'\omega' k'(v)\}\Psi(u; v), \qquad k'(v) = \zeta(v) - v\frac{\eta'}{\omega'}. \tag{2.9}$$

2.2. Normalization of the Bloch function of one-gap potentials

Since normalization of the BF plays an important role in the construction of the WF (see the next section), we shall show how to compute the normalization constant, although this question has been considered in chapter VIII of [2].

We normalize the BF according to

$$2\pi\langle|\Psi(x, E)|^2\rangle = 1, \tag{2.10}$$

where

$$\langle f(x)\rangle = \lim_{L\to\infty}\frac{1}{L}\int_{-L/2}^{L/2} f(x)\,\mathrm{d}x.$$

The following proposition is valid.

Proposition 2.1. *Normalized Bloch functions of elliptic one-gap potentials are of the form*

$$\Psi(x; \alpha) = -\frac{\mathrm{i}}{(2\pi)^{1/2}}\left[-\wp(v) - \frac{\eta'}{\omega'}\right]^{-1/2}\frac{\sigma(v-u)}{\sigma(v)\sigma(u)}\exp\{v\eta + (u-\omega)\zeta(v)\}, \tag{2.11}$$

where $u = \mathrm{i}x + \omega, x \in \mathbb{R}; v = \alpha + \omega', \alpha \in \mathbb{R}$.

Proof. Let us denote the normalized BF as

$$\Psi(u; v) = C(v)\Phi(u; v),$$

where $\Phi(u; v)$ is the non-normalized BF given by

$$\Phi(u; v) = \frac{\sigma(v-u)}{\sigma(v)\sigma(u)}\mathrm{e}^{(u-\omega)\zeta(v)},$$

and $C(v)$ is the normalization constant defined by equation (2.10):

$$2\pi\frac{|C(v)|^2}{2\omega'}\int_{\omega}^{\omega+2\omega'}|\Phi(u;v)|^2\,\mathrm{d}u = 1.$$

The complex conjugated (non-normalized) BF is

$$\begin{aligned}\overline{\Phi}(u;v) &= \frac{\overline{\sigma}(v-u)}{\overline{\sigma}(v)\overline{\sigma}(u)}\mathrm{e}^{-(u-\omega)\overline{\zeta}(v)} = \frac{\sigma(\overline{v}-\overline{u})}{\sigma(\overline{v})\sigma(\overline{u})}\mathrm{e}^{-(u-\omega)\zeta(\overline{v})}\\ &= -\frac{\sigma(v-2\omega'+u-2\omega)}{\sigma(v-2\omega')}\sigma(u-2\omega)\mathrm{e}^{(u-\omega)\zeta(v-2\omega')}\\ &= \frac{\sigma(v+u)}{\sigma(v)\sigma(u)}\mathrm{e}^{-(v-\omega')2\eta-(u-\omega)\zeta(v)},\end{aligned}$$

where the following elementary equalities were used:

$$\begin{aligned}&\overline{\sigma}(z)=\sigma(\overline{z}), \qquad \overline{\zeta}(z)=\zeta(\overline{z}), \qquad \overline{(u-\omega)}=-(u-\omega),\\ &\overline{u}=-u+2\omega, \qquad \overline{v}=v-2\omega',\\ &\zeta(v-2\omega')=\zeta(v)-2\eta',\\ &\sigma(v-2\omega')=-\sigma(v)\exp(-(v-\omega')2\eta'),\\ &\sigma(u-2\omega)=-\sigma(u)\exp(-(u-\omega)2\eta).\end{aligned}$$

By multiplying the above expressions of $\Phi(u;v)$ and $\overline{\Phi(u;v)}$, we get

$$|\Phi(u;v)|^2 = \frac{\sigma(v-u)\sigma(v+u)}{\sigma^2(v)\sigma^2(u)}\,\mathrm{e}^{-(v-\omega')2\eta} = [\wp(u)-\wp(v)]\,\mathrm{e}^{(v-\omega')2\eta},$$

where, in the last step, we have used the well-known formula

$$\frac{\sigma(v-u)\sigma(v+u)}{\sigma^2(v)\sigma^2(u)} = \wp(u)-\wp(v).$$

The normalization condition can be then written in the form

$$\begin{aligned}1 &= 2\pi\frac{|C(v)|^2}{2\omega'}\int_{\omega}^{\omega+2\omega'}[\wp(u)-\wp(v)]\,\mathrm{e}^{(v-\omega')2\eta}\,\mathrm{d}u\\ &= 2\pi|C(v)|^2\left[-\frac{\eta'}{\omega'}-\wp(v)\right]\mathrm{e}^{-(v-\omega')2\eta},\end{aligned}$$

since

$$\frac{1}{2\omega'}\int_{\omega}^{\omega+2\omega'}\wp(u)\,\mathrm{d}u = \frac{1}{2\omega'}[\zeta(\omega)-\zeta(\omega+2\omega')] = -\frac{\eta'}{\omega'}.$$

Thus we have obtained, for the normalization constant, the expression

$$C(v) = \frac{\mathrm{e}^{\mathrm{i}\theta}}{(2\pi)^{1/2}}\left[-\frac{\eta'}{\omega'}-\wp(v)\right]^{-1/2}\mathrm{e}^{(v-\omega')\eta}, \tag{2.12}$$

with an arbitrary phase factor $\exp(\mathrm{i}\theta)$, $\theta \in \mathbb{R}$. In the following, we fix this factor as

$$\exp(\mathrm{i}\theta) = \exp\left(\omega'\eta - \frac{\mathrm{i}\pi}{2}\right). \qquad \square$$

Next, we shall show that this choice of the phase leads to the WF that is both real and symmeteric about $x = 0$. Moreover, this choice of the phase is unique (see section 6 of [7]).

The normalized BF $\Psi(u; v)$ satisfy a number of useful properties under the action of symmetry operations. For centro-symmetrical potentials, the transformation $x \to -x$ of the lattice corresponds to a transformation in the Jacobian $u \to \hat{u} = -u + 2\omega$, and the following propositions can be proved.

Proposition 2.2.

$$\Psi(\hat{u}; v) = \Psi(-u + 2\omega; v) = \overline{\Psi}(u; v).$$

Proof.

$$\begin{aligned}\Psi(\hat{u}; v) &= \Psi(-u + 2\omega; v)\\ &= \mathrm{i}(2\pi)^{-1/2}\left[-\wp(v) - \frac{\eta'}{\omega'}\right]^{-1/2} \frac{\sigma(v + u - 2\omega)}{\sigma(v)\sigma(u - 2\omega)} \exp[v\eta - (u - \omega)\zeta(v)]\\ &= \mathrm{i}(2\pi)^{-1/2}\left[-\wp(v) - \frac{\eta'}{\omega'}\right]^{-1/2} \frac{\sigma(v + u)}{\sigma(v)\sigma(u)} \exp[-v\eta - (u - \omega)\zeta(v)] = \overline{\Psi}(u; v). \qquad \square\end{aligned}$$

Similarly, the transformation $\alpha \to -\alpha$ corresponds to $v \to \hat{v} = -v + 2\omega'$, and the following proposition is valid.

Proposition 2.3.

$$\Psi(u; \hat{v}) = \Psi(u; -v + 2\omega') = \overline{\Psi}(u; v).$$

Proof.

$$\begin{aligned}\Psi(u; \hat{v}) &= \Psi(u; -v + 2\omega')\\ &= -\mathrm{i}(2\pi)^{-1/2}\left[-\wp(v) - \frac{\eta'}{\omega'}\right]^{-1/2} \frac{\sigma(-v - u + 2\omega')}{\sigma(-v + 2\omega')\sigma(u)}\\ &\quad\times \exp[(-v + 2\omega')\eta + (u - \omega)\zeta(v - 2\omega')]\\ &= -\mathrm{i}(2\pi)^{-1/2}\left[-\wp(v) - \frac{\eta'}{\omega'}\right]^{-1/2} \frac{\sigma(v + u)}{\sigma(v)\sigma(u)} \exp[-v\eta - (u - \omega)\zeta(v)]\\ &= \overline{\Psi}(u; v). \qquad \square\end{aligned}$$

The above propositions can be used to study the elementary properties of the BF, $\Psi(x;k) \equiv \Psi(u(x); v(k))$, where $u(x) = \mathrm{i}x + \omega$ and $v(k)$ is the inverse of the function $k(v) = \zeta(v) - (\eta'/\omega')v$. In this regard, note that

$$x(\hat{u}) = -x(u), \qquad k(\hat{v}) = -k(v).$$

The following two properties are easily proved.

Property 1. $\Psi(-x;k) = \overline{\Psi}(x;k)$.

Proof.

$$\Psi(-x;k) = \Psi(\hat{u}, v) = \overline{\Psi}(u;v) = \overline{\Psi}(x;k). \qquad \square$$

Property 2. $\Psi(x;-k) = \overline{\Psi}(x;k)$.

Proof.

$$\Psi(x;-k) = \Psi(u;\hat{v}) = \overline{\Psi}(u;v) = \overline{\Psi}(x;k). \qquad \square$$

3. Analytical properties of the Wannier function of elliptic one-gap potentials

3.1. Definition and basic properties

In 1937, Wannier [6] introduced a complete set of functions for an electron in a lattice structure. The WF, $W_n(x)$, are defined as

$$W_n(x) = \left(\frac{T}{2\pi}\right)^{1/2} \int_{-\pi/T}^{\pi/T} \Psi_n(x;k)\,\mathrm{d}k, \tag{3.1}$$

where the integral is made on the Brillouin zone. WF for the Schrödinger operator with periodic potential $U(x), U(x-mT)$, $m \in \mathbb{Z}$, are localized linear combinations of all the Bloch eigenstates of a given nth spectral band. One can easily prove that if the BF is normalized according to equation (2.10), then the WF is normalized on the full line,

$$\int_{-\infty}^{\infty} |W_n(x)|^2\,\mathrm{d}x = 1.$$

Using the translation operator, one then constructs a countable set of WF: $W_n^{(l)}(x) := W_n(x-lT)$, $l \in \mathbb{Z}$ which is complete and forms an orthonormal basis

$$\int_{-\infty}^{\infty} \overline{W}_n^{(l)}(x) W_{n'}^{(l')}(x)\,\mathrm{d}x = \delta_{nn'}\delta_{ll'}, \quad l \in \mathbb{Z}.$$

The inverse transformation allows us to express a BF in terms of WF as

$$\Psi_n(x;k) = \left(\frac{T}{2\pi}\right)^{1/2} \sum_{l=-\infty}^{\infty} W_n^{(l)}(x)\,\mathrm{e}^{\mathrm{i}lak}. \tag{3.2}$$

In the following, we shall omit the band index n since we deal only with one band. Properties of WF of one-dimensional periodic potentials were studied by Kohn [7], where he proved that for every band there exists one and only one WF that satisfies simultaneously the following three properties: (i) $\overline{W}(x) = W(x)$; (ii) $W(-x) = \pm W(x)$; (iii) $W(x) = \mathrm{O}(\exp(-h|x|))$, where $h > 0$. In the following, we investigate the analytical properties of the WF for the one-gap potential in equation (2.1). In this case, the WF is given by the formula

$$
\begin{aligned}
W(x) &= \left(\frac{T}{2\pi}\right)^{1/2} \int_{-\pi/T}^{\pi/T} \Psi(x;k)\,\mathrm{d}k \\
&= \left(\frac{T}{2\pi}\right)^{1/2} \left(\int_{-\pi/T}^{0} + \int_{0}^{\pi/T}\right) \Psi(x;k)\,\mathrm{d}k \\
&= \left(\frac{T}{2\pi}\right)^{1/2} \int_{0}^{\pi/T} (\Psi(x;k) + \Psi(x;-k))\,\mathrm{d}k \\
&= \left(\frac{T}{2\pi}\right)^{1/2} 2\mathrm{Re} \int_{0}^{\pi/T} \Psi(x;k)\,\mathrm{d}k \\
&= \mathrm{Re}\left\{-\mathrm{i}\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi} \int_{\omega'}^{\omega+\omega'} \sqrt{\frac{\mathrm{d}k(v)}{\mathrm{d}v}}\, \frac{\sigma(v-u)}{\sigma(v)\sigma(u)}\, \mathrm{e}^{v\eta + (u-\omega)\zeta(v)}\,\mathrm{d}v\right\}.
\end{aligned} \tag{3.3}
$$

Using the properties of the BF, $\Psi(x;k)$, the following basic properties of the WF can be proved.

Proposition 3.1. $\overline{W}(x) = W(x)$.

Proof.

$$
\overline{W}(x) = \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_{0}^{\pi/T} \overline{\Psi}(x;k)\,\mathrm{d}k = \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_{0}^{\pi/T} \Psi(x;k)\,\mathrm{d}k = W(x). \qquad \square
$$

Proposition 3.2. $W(-x) = W(x)$.

Proof.

$$
\begin{aligned}
W(-x) &= \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_{0}^{\pi/T} \Psi(-x;k)\,\mathrm{d}k = \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_{0}^{\pi/T} \overline{\Psi}(x;k)\,\mathrm{d}k \\
&= \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_{0}^{\pi/T} \Psi(x;k)\,\mathrm{d}k = W(x). \qquad \square
\end{aligned}
$$

3.2. Power series expansion of the WF at $x = 0$

We shall construct in this section the power series expansion of the WF of one-gap potential.

Theorem 3.3. *The WF of the lower energy band for the one-gap potential admits the following power series representation:*

$$
W(x) = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!} W_{2p} x^{2p}, \tag{3.4}
$$

where the coefficients W_{2p} *of the expansion* (3.4) *are given by the formula*

$$W_{2p} = \sum_{l=0}^{p} M_l q_{p,l}. \tag{3.5}$$

Here

$$M_l = \frac{\sqrt{2\mathrm{i}}}{\pi}\sqrt{\omega' e_3 + \eta'} \sum_{j=0}^{l} \frac{(2j-1)!!l!}{2^j (j!)^2 (l-j)!} e_3^j (e_2 - e_3)^{l-j} \times F\left(-\frac{1}{2}, j+\frac{1}{2}; j+1; \frac{\omega'(e_3 - e_2)}{\omega' e_3 + \eta'}\right), \tag{3.6}$$

where $F(a, b; c; z)$ *is the standard hypergeometric function,* e_2, e_3 *are branch points of the elliptic curve and* $q_{p,l}$ *are coefficients of polynomials in* $\wp(v)$

$$Q_p(\wp(v)) = \sum_{l=0}^{p} q_{p,l}\wp^l(v)$$

defined by the recurrence

$$Q_p(\wp(v)) = \sum_{m=0}^{p-1} \binom{2p}{2m-2} \phi_{m-p-1} Q_m(\wp(v)) \tag{3.7}$$

with

$$\phi_0 = 2e_1 + \wp(v), \qquad \phi_p = 2\wp^{(2p)}(\omega).$$

The first few coefficients of the expansion (3.4) *are*

$$\begin{aligned} W_0 &= M_0, \\ W_2 &= M_1 + 2e_1 M_0, \\ W_4 &= M_2 + 4e_1 M_1 + (4e_1^2 + 2\wp''(\omega))M_0, \\ W_6 &= M_3 + 6e_1 M_2 + (14\wp''(\omega) + 12e_1^2)M_1 + (2\wp^{(IV)}(\omega) + 28\wp''(\omega)e_1 + 8e_1^3)M_0. \end{aligned} \tag{3.8}$$

Proof. We have

$$W(x) = \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_0^{\pi/T} \Psi(x; k)\,\mathrm{d}k. \tag{3.9}$$

Because the BF $\Psi(x; k)$ is even in x, we can write it in the form of the Taylor expansion

$$\Psi(u, v) = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!} \Psi_{2p}(v) x^{2p}, \tag{3.10}$$

where

$$\Psi_{2p}(v) = \left[\frac{\mathrm{d}^{2p}}{\mathrm{d}u^{2p}}\Psi(u, v)\right]_{u=\omega}, \quad p = 1, \ldots .$$

If we substitute the Taylor expansion (3.10) into (3.9), we obtain the expansion (3.4) with the following coefficients:

$$W_{2p} = \left(\frac{2T}{\pi}\right)^{1/2} \mathrm{Re} \int_0^{\pi/T} \Psi_{2p}(v)\,\mathrm{d}k. \tag{3.11}$$

Using the Schrödinger equation, we obtain easily, for the $\Psi_{2p}(v)$, a recurrent relation

$$\Psi_{2p}(v) = \sum_{l=0}^{p-1} \binom{2p}{2l-2} \phi_{p-l-1} \Psi_{2l}(v),$$

$$\phi_0 = 2e_1 + \wp(v), \qquad \phi_p = 2\wp^{(2p)}(\omega).$$

The form of this relation leads to the conclusion that

$$\Psi_{2p}(v) = Q_p(\wp(v))\Psi_0(v),$$

where

$$\Psi_0(v) = \Psi(\omega; v) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\wp(v) - e_1}{\wp(v) + \eta'/\omega'}} \tag{3.12}$$

and $Q_p(\wp(v))$ are polynomials of the pth order in $\wp(v)$, given by

$$Q_p(\wp(v)) = \sum_{l=0}^{p} q_{p,l}\wp^l(v).$$

As for $\Psi_{2p}(v)$, the polynomials $Q_p(\wp(v))$ satisfy the following recurrent relation:

$$Q_p(\wp(v)) = \sum_{m=0}^{p-1} \binom{2p}{2m-2} \phi_{m-p-1} Q_m(\wp(v)) \tag{3.13}$$

with

$$\phi_0 = 2e_1 + \wp(v), \qquad \phi_p = 2\wp^{(2p)}(\omega).$$

In particular, the first few polynomials $Q_p(\wp(v))$ are

$$\begin{aligned} Q_1(\wp(v)) &= \wp(v) + 2e_1, \\ Q_2(\wp(v)) &= \wp(v)^2 + 4e_1\wp(v) + 2\wp''(\omega) + 4e_1^2, \\ Q_3(\wp(v)) &= \wp(v)^3 + 6e_1\wp(v)^2 + (14\wp''(\omega) + 12e_1^2)\wp(v) + 2\wp^{(IV)}(\omega) + 28e_1\wp''(\omega) + 8e_1^3. \end{aligned} \tag{3.14}$$

Next, we calculate the integral expressions of the coefficients W_{2p}. We show that the following formula is valid:

$$\begin{aligned} M_l &= -2\left(\frac{\omega'}{\mathrm{i}\pi}\right)^{1/2} \int_0^{\omega'} \wp(v)^l \left(\wp(v) + \frac{\eta'}{\omega'}\right) \Psi(\omega; v)\,\mathrm{d}v \\ &= \left(\frac{2T}{\pi}\right)^{1/2} \int_0^{\omega'} \wp(v)^l \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\wp(v) - e_1}{\wp(v) + (\eta'/\omega')}} \left(-\wp(v) - \frac{\eta'}{\omega'}\right) \mathrm{d}v \\ &= \frac{T^{1/2}}{\pi} \int_0^{\omega'} \wp(v)^l \sqrt{\wp(v) - e_1} \sqrt{\wp(v) + \frac{\eta'}{\omega'}}\,\mathrm{d}v. \end{aligned}$$

After the substitution $\wp(v) = s$, the computation is reduced to the derivation of the complete elliptic integral

$$M_l = -\frac{\sqrt{-\mathrm{i}\omega'}}{\pi}\int_{e_3}^{e_2} s^l \sqrt{\frac{s+(\eta'/\omega')}{(s-e_2)(s-e_3)}}\,\mathrm{d}s. \tag{3.15}$$

By introducing a new variable

$$t = \frac{s-e_3}{e_2-e_3},$$

the integral M_l acquires the form

$$M_l = -\frac{\sqrt{-\mathrm{i}\omega'}}{\pi}\sqrt{e_2-e_3}\int_0^1 ((e_2-e_3)t-e_3)^l \sqrt{\frac{1-\widetilde{k}^2 t}{t(1-t)}}\,\mathrm{d}t, \tag{3.16}$$

where

$$\widetilde{k} = \sqrt{\frac{\omega'(e_3-e_2)}{\omega' e_3+\eta'}} \tag{3.17}$$

is the Jacobi modulus of the elliptic curve

$$Y^2 = (X-e_2)(X-e_3)\left(X+\frac{\eta'}{\omega'}\right). \tag{3.18}$$

Using the integral representation of the hypergeometric function (see e.g. [18])

$$F(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}}{(1-tz)^a}\,\mathrm{d}t, \tag{3.19}$$

we obtain the required expression

$$M_l = \frac{\sqrt{2\mathrm{i}}}{\pi}\sqrt{\omega' e_3+\eta'}\sum_{j=0}^{l}\frac{(2j-1)!!l!}{2^j(j!)^2(l-j)!}e_3^j(e_2-e_3)^{l-j}$$
$$\times F\left(-\frac{1}{2}, j+\frac{1}{2}; j+1; \widetilde{k}^2\right). \tag{3.20}$$

□

It is worth noting that the coefficient W_0 gives an exact value of the amplitude of WF at the localization site $x = 0$,

$$W_0 = \frac{\sqrt{2\mathrm{i}}}{2}\sqrt{\omega' e_3+\eta'}\,F\left(-\frac{1}{2},\frac{1}{2};1;\widetilde{k}^2\right). \tag{3.21}$$

This amplitude can also be written in the alternative form

$$W_0 = \frac{\sqrt{2\mathrm{i}}}{\pi}\sqrt{\omega' e_3+\eta'}\,E(\widetilde{k}), \tag{3.22}$$

where $E(\widetilde{k})$ is the complete integral of the second kind depending on $\widetilde{k}$. Also note that, by using the relations

$$\left(z\frac{\mathrm{d}}{\mathrm{d}z}+b\right) = bF(a,b+1;c;z),$$

$$\left[(1-z)\frac{\mathrm{d}}{\mathrm{d}z}+c-a-b\right]F(a,b;c;z) = \frac{(c-a)(c-b)}{c}F(a,b;c+1;z),$$

one can express all the hyperegeometric functions $F(-\frac{1}{2}, j+\frac{1}{2}; j+1; \widetilde{k}^2)$ in (3.20) in terms of the derivatives of $F(-\frac{1}{2}, \frac{1}{2}; 1; \widetilde{k}^2)$ with respect to $\widetilde{k}^2$, and therefore the whole expression can be written in terms of the complete integral $E(\widetilde{k})$ and its derivatives.

We remark that the quantities $\wp^{(2j)}(\omega)$, $j = 1, \ldots,$ can be computed in a recurrent way, examples of the first of them being [18]

$$\wp''(\omega) = 3!\left(e_1^2 - \frac{1}{2^2 \cdot 3} g_2\right),$$

$$\wp^{(IV)}(\omega) = 5!\left(e_1^3 - \frac{3}{2^2 \cdot 5} g_2 e_1 - \frac{1}{2 \cdot 5} g_3\right),$$

$$\wp^{(VI)}(\omega) = 7!\left(e_1^4 - \frac{1}{5} g_2 e_1^2 - \frac{1}{7} g_3 e_1 + \frac{1}{2^4 \cdot 5 \cdot 7} g_2^2\right).$$

3.3. Asymptotic expansion of the WF

In this section, we obtain the asymptotic expression for the WF at $x \to +\infty$ by the steepest descents method. This method (see e.g. [19]) permits us to compute the asymptotic expression of integrals of the type

$$F(x) = \int_\gamma f(z) \exp\{x S(z)\}\, \mathrm{d}z,$$

where γ is a contour in the complex plane, and the functions $f(z)$ and $S(z)$ are holomorphic in the vicinity of γ. When a saddle point z_0, defined by the equation

$$\frac{\mathrm{d}}{\mathrm{d}z} S(z_0) = 0,$$

does not coincide with the edges of the contour, the asymptotic formula of the integral $F(x)$ reads

$$F(x) = \sqrt{-\frac{2\pi}{x \mathrm{d}^2 S(z_0)/\mathrm{d}z^2}} \exp\{x S(z_0)\}[f(z_0) + \mathrm{O}(x^{-1})].$$

In our case, we must use a non-standard variant of the steepest descents method, since the exponential in the integrand will have the form $xS(z)$ only at $|x| \to +\infty$ and $f(z_0) = 0$.

Proposition 3.4. *At $x \to \infty$, the WF of the lower energy band for the one-gap potential has the following asymptotic expression:*

$$W(x) \simeq \mathrm{Re}\left\{\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi}\left(e_1 + \frac{\eta'}{\omega'}\right)^{1/2} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)}\, \mathrm{e}^{(u-\omega)\zeta(v)} \left[\frac{\mathrm{i}}{2\wp'(v)}\right]^{1/4} \frac{\Gamma(3/4)}{x^{3/4}}\right\}, \qquad (3.23)$$

where v is a solution of the equation

$$\wp(v) = -\frac{\eta'}{\omega'} \quad \textit{or} \quad k'(v) = 0, \qquad (3.24)$$

such that the complex number $\omega' k(v) = \omega'(\zeta(v) - (\eta'/\omega')v)$ *has a negative real part. This means that*

$$W(x) \simeq \exp(-h|x|)|x|^{-3/4}, \quad |x| \to \infty,$$

where $h = |k(v)|$ *and* v *is defined by the equation* $k'(v) = 0$.

Proof. We use the expression of the WF for the first energy band $[e_3, e_2]$ given in equation (3.3). Since

$$\begin{aligned}\frac{\sigma(v-u)}{\sigma(v)\sigma(u)} &= -\frac{\sigma(u-v)}{\sigma(\omega-v)}\frac{\sigma(\omega)}{\sigma(u)}\frac{\sigma(\omega-v)}{\sigma(v)\sigma(\omega)}\\ &= \frac{\sigma(v-\omega)}{\sigma(v)\sigma(\omega)}\exp\left\{\int_\omega^u [\zeta(s-v)-\zeta(s)]\,\mathrm{d}s\right\}\\ &= [\wp(v)-e_1]^{1/2}\exp\left\{-v\eta+\int_\omega^u [\zeta(s-v)-\zeta(s)]\,\mathrm{d}s\right\},\end{aligned}$$

we have that equation (3.3) can be rewritten as

$$W(x) = \mathrm{Re}\left\{\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi}\int_{\omega'}^{\omega+\omega'}[e_1-\wp(v)]^{1/2}\sqrt{\frac{\mathrm{d}k(v)}{\mathrm{d}v}}\right.$$
$$\left.\times\exp\left\{\int_\omega^u [\zeta(s-v)-\zeta(s)+\zeta(v)]\,\mathrm{d}s\right\}\mathrm{d}v\right\}. \tag{3.25}$$

When $x \to +\infty$, we can calculate the integral in equation (3.25) by the steepest descents method. In this regard, we remark that the argument of the exponential, as a function of v, has saddle points which are defined by the equation

$$\frac{\mathrm{d}}{\mathrm{d}v}\int_\omega^u [\zeta(s-v)-\zeta(s)+\zeta(v)]\,\mathrm{d}s = 0,$$

or, in other words, by the equation

$$\wp(v) = -\frac{\zeta(u-v)-\zeta(\omega-v)}{u-\omega}.$$

At $x \to +\infty$, the last equation attains the form (3.24). Since $\overline{\wp}(v) = \wp(\overline{v})$, we have that if v is a saddle point then $\overline{v}$ is also a saddle point. On the other hand, $\wp(v)$ is an elliptic function of the second order, so it takes every value twice in the fundamental domain, implying that there are two saddle points, say v_1, v_2, in the fundamental domain. The sum of the values v_1, v_2 must be a period of the lattice, which in our case means that $v_1 + v_2 = 2(\omega + \omega')$. It is not difficult to show that

$$v_1 = \omega + \omega' + \mathrm{i}\beta, \qquad v_2 = \omega + \omega' - \mathrm{i}\beta, \quad \beta \in \mathbb{R},$$

i.e. the two saddle points v_1, v_2 are situated in the spectral gap. The periodicity of the Weierstrass function $\wp(z)$ in the complex plane give rise to a countable set V of saddle points,

$$V = \{v_1 + 2n_1\omega', v_2 + 2n_2\omega' : n_1, n_2 \in \mathbb{Z}\}.$$

In order to build the proper asymptotic expression for the Wannier function $W(x)$, we must select from this set a special saddle point which we denote by v_0. In the neighbourhood of v_0, we have

$$\sqrt{\frac{\mathrm{d}k(v)}{\mathrm{d}v}} \simeq [-\wp'(v_0)]^{1/2}(v-v_0)^{1/2},$$

$$\begin{aligned}\int_\omega^u [\zeta(s-v)-\zeta(s)+\zeta(v)]\,\mathrm{d}s &\simeq \int_\omega^u [\zeta(s-v_0)-\zeta(s)+\zeta(v_0)]\,\mathrm{d}s\\ &+\frac{1}{2}(v-v_0)^2\int_\omega^u [\zeta''(s-v_0)+\zeta''(v_0)]\,\mathrm{d}s = \int_\omega^u [\zeta(s-v_0)-\zeta(s)+\zeta(v_0)]\,\mathrm{d}s\\ &-(u-\omega)\frac{1}{2}\left[\wp'(v_0)+\frac{\wp(u-v_0)-\wp(\omega-v_0)}{u-\omega}\right](v-v_0)^2\\ &\simeq \int_\omega^u [\zeta(s-v_0)-\zeta(s)+\zeta(v_0)]\,\mathrm{d}s-(u-\omega)\frac{1}{2}\wp'(v_0)(v-v_0)^2.\end{aligned}$$

Substituting the last two expressions into the integral representation of the WF in (3.25), we obtain

$$\begin{aligned}W_0(x) &\simeq \mathrm{Re}\left\{\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi}\left(e_1+\frac{\eta'}{\omega'}\right)^{1/2}\exp\left\{\int_\omega^u [\zeta(s-v_0)-\zeta(s)+\zeta(v_0)]\,\mathrm{d}s\right\}\right.\\ &\quad\left.\times\int_{C_0}\mathrm{d}v\,[-\wp'(v_0)]^{1/2}(v-v_0)^{1/2}\exp\left\{-\frac{1}{2}(u-\omega)\wp'(v_0)(v-v_0)^2\right\}\right\}\\ &= \mathrm{Re}\left\{\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi}\left(e_1+\frac{\eta'}{\omega'}\right)^{1/2}\frac{\sigma(v_0-u)}{\sigma(v_0)\sigma(u)}\exp\{(u-\omega)\zeta(v_0)\}\right.\\ &\quad\left.\times\int_{C_0}\mathrm{d}r\,[-\wp'(v_0)]^{1/2}r^{1/2}\exp\left\{-\frac{1}{2}(u-\omega)\wp'(v_0)r^2\right\}\right\},\end{aligned}$$

where C_0 is a contour passing through the saddle point v_0. The integral in the last expression can be calculated as

$$\begin{aligned}I_0 &= \int_{C_0}\mathrm{d}r\,[-\wp'(v_0)]^{1/2}r^{1/2}\exp\left\{-\frac{1}{2}(u-\omega)\wp'(v_0)r^2\right\}\\ &= \left[\frac{\mathrm{i}}{2\wp'(v_0)}\right]^{1/4}\frac{1}{x^{3/4}}\int_0^\infty \mathrm{e}^{-t}t^{-1/4}\,\mathrm{d}t = \left[\frac{\mathrm{i}}{2\wp'(v_0)}\right]^{1/4}\frac{\Gamma(3/4)}{x^{3/4}}.\end{aligned}$$

Notice that, since $\wp'(v_0) = -2[\wp(v_0)-e_1]^{1/2}[\wp(v_0)-e_2]^{1/2}[\wp(v_0)-e_3]^{1/2}$ and $e_3 \leqslant e_2 \leqslant \wp(v_0) \leqslant e_1$, we have that $\wp'(v_0) = -\mathrm{i}|\wp'(v_0)|$.

For the function $W_0(x)$, we finally obtain

$$\begin{aligned}W_0(x) &\simeq \mathrm{Re}\left\{\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi}\left(e_1+\frac{\eta'}{\omega'}\right)^{1/2}\left[\frac{\mathrm{i}}{2\wp'(v_0)}\right]^{1/4}\frac{\Gamma(3/4)}{x^{3/4}}\right.\\ &\quad\left.\times\exp\left\{\int_\omega^u [\zeta(s-v_0)-\zeta(s)+\zeta(v_0)]\,\mathrm{d}s\right\}\right\}\\ &= \mathrm{Re}\left\{\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi}\left(e_1+\frac{\eta'}{\omega'}\right)^{1/2}\frac{\sigma(v_0-u)}{\sigma(v_0)\sigma(u)}\mathrm{e}^{(u-\omega)\zeta(v_0)}\left[\frac{\mathrm{i}}{2\wp'(v_0)}\right]^{1/4}\frac{\Gamma(3/4)}{x^{3/4}}\right\}.\end{aligned}$$

The asymptotic behaviour of the function $W_0(x)$ at $x \to +\infty$ is defined by the factor

$$f(u, v_0) = \frac{\sigma(v_0 - u)}{\sigma(u)} \exp[(u - \omega)\zeta(v_0)],$$

which satisfies the relation

$$f(u + 2n\omega', v_0) = f(u, v_0) \exp\left[2n\omega'\left(\zeta(v_0) - \frac{\eta'}{\omega'} v_0\right)\right] = f(u, v_0) \exp[2n\omega' k(v_0)].$$

The saddle point v_0 must be chosen in such a manner that the complex number $\omega' k(v_0)$ has a negative real part. From previous considerations, it follows that the point $\overline{v}_0$ is also a saddle point. The asymptotic behaviour of the function $W_0(x)$ at $x \to -\infty$ is defined by this saddle point, which corresponds to the complex number $\omega' k(\overline{v}_0) = \omega'(\zeta(\overline{v}_0) - (\eta'/\omega')\overline{v}_0)$ with a positive real part. □

It is appropriate to make here some remarks.

According to the theorem,

$$W(x) \simeq \exp(-|x||k(\alpha_0)|)|x|^{-3/4}, \quad |x| \to \infty.$$

It is easy to understand such an asymptotic behaviour of the WF at $|x| \to \infty$ if we take into account that

$$W(x) \simeq \mathrm{Re}\left\{\int_C (k - k_0)^\beta \mathrm{e}^{\mathrm{i}kx}\right\} \simeq 2\sin(\beta\pi)\,\Gamma(1 + \beta)x^{-(1+\beta)}\mathrm{e}^{-\mathrm{Im}\,k_0 x},$$

where k_0 is a branching point of the energy $E(k)$, and that, due to a normalization constant of the wave function,

$$\Psi(k) \simeq (k - k_0)^{-1/4},$$

the equality $\beta = -1/4$ is valid. As far as we know, this asymptotic law was mentioned for the first time in [10].

It is of interest to note also that the equation

$$\wp(v) + \frac{\eta'}{\omega'} = 0$$

has, obviously, the following solution:

$$v = \pm \int_{-(\eta'/\omega')}^{\infty} \frac{\mathrm{d}x}{\sqrt{4x^3 - g_2 x - g_3}}.$$

The more general problem to solve the equation

$$\wp(v, \omega, \omega') = c(\omega, \omega'),$$

is a well-known mathematical problem in the theory of elliptic functions. A solution of the problem in terms of Eisenstein series is presented in [20].

In the above theorem, we have obtained results for the WF of a lower energy band. Results for the WF of a higher band,

$$W(x) = \mathrm{Re}\left\{-\mathrm{i}\frac{\sqrt{-2\mathrm{i}\omega'}}{\pi} \int_\omega^{\widetilde{\omega}} \sqrt{\frac{\mathrm{d}k(v)}{\mathrm{d}v}} \frac{\sigma(v - u)}{\sigma(v)\sigma(u)} \mathrm{e}^{v\eta + (u-\omega)\zeta(v)}\,\mathrm{d}v\right\},$$
$$k(\widetilde{\omega}) = \zeta(\widetilde{\omega}) - \frac{\eta'}{\omega'}\widetilde{\omega} = \frac{\pi}{T}, \tag{3.26}$$

are similar to the ones presented above and, as a result, we omit appropriate considerations.

Let us now discuss two limiting cases. The limit $\tau = \omega'/\omega \to 0$ corresponds to the free electron case or the empty lattice case. In this limit, the energy gap is zero, $e_1 = e_2$, there are no saddle points and, as a result, we have the well-known free electron WF,

$$W(x) = \frac{T^{1/2}}{\pi x} \sin\left(\frac{\pi x}{T}\right).$$

The limit $\tau = \omega'/\omega \to \mathrm{i}\infty$ corresponds to the case of tightly bound electrons. In this case, the width of the lower energy band is zero, $e_2 = e_3$, and the appropriate wave function is as follows:

$$\Psi(x) = \left(\frac{\alpha}{2}\right)^{1/2} \frac{1}{\cosh \alpha x}, \qquad E_0 = -\alpha^2,$$

where E_0 is the binding energy. The wave functions of higher energy bands are of the form

$$\Psi(x,k) = \frac{1}{\sqrt{2\pi}\sqrt{k^2+\alpha^2}} (|k| + \mathrm{i}\alpha \tanh(\alpha x))\, \mathrm{e}^{\pm \mathrm{i}kx}, \qquad E = k^2.$$

In section 4, we shall compare our analytical results with numerical ones.

4. Approximate analytical expressions of WF and the numerical results

The results of the previous section permit us to construct the following approximate expression of the WF for one-gap potentials:

$$\begin{aligned} W(x) &= W_0 + W_2 x^2 + W_4 x^4 + W_6 x^6 \quad \text{for } |x| \leqslant x_0 \\ &= \mathrm{Re}\left\{ \frac{\sqrt{-2\mathrm{i}\omega'}}{\pi} \left(e_1 + \frac{\eta'}{\omega'}\right)^{1/2} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} \right. \\ &\quad \left. \times \exp\{(u-\omega)\zeta(v)\} \left[\frac{\mathrm{i}}{2\wp'(v)}\right]^{1/4} \frac{\Gamma(3/4)}{x^{3/4}} \right\} \quad \text{for } |x| > x_0, \end{aligned} \tag{4.1}$$

where $u = \mathrm{i}x + \omega$, $v = v_+ + \omega'$, the coefficients $W_0, \ldots, W_6$ are given by formulae (3.8) and the point x_0 is chosen so as to satisfy the normalization condition $\|W(x)\|^2 = 1$.

To check the validity of this expression, we shall compare the WF obtained from equation (4.1) with the one obtained directly from definition (3.1) by numerical methods, using the expression of the normalized BF in proposition 2.1. In figure 1, we show the band structure obtained for the one-gap potential with parameter values $e_1 = 2, e_2 = -0.5, e_3 = -1.5$, while in figure 2, we depict the WF associated to the lower band. We see that the agreement between the analytical approximation and direct numerical calculations is excellent both in the proximity of the origin and far away from it, these being the regions of validity of the corresponding expansions. In the intermediate region, however, some discrepancy appears. It is possible that, for some set of potential parameters, the validity regions of the two expansions (near the origin and far from the origin) can overlap at some point x_0 so that it is possible to join them to the single smooth analytical approximation (4.1), which stay close to the exact numerical curve in the whole spatial domain. The existence of a point of this kind is possible only for one-gap potentials. Such a good matching of two expansions is shown in figure 3, where the WF of the lower band for a potential with another set of parameters is depicted.

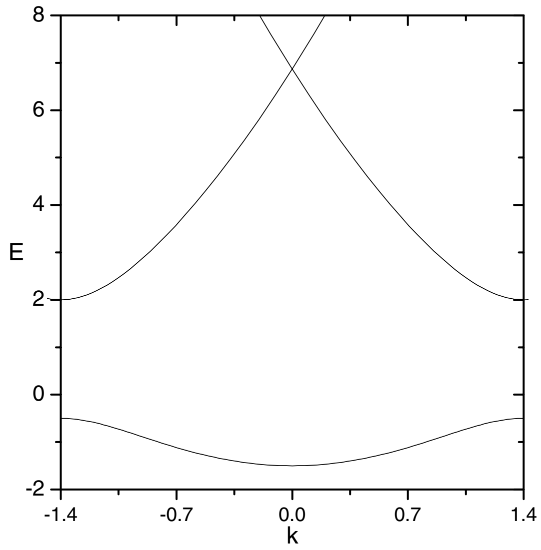

Figure 1. Energy bands of the one-gap potential with parameters of the elliptic curve $e_1 = 2, e_2 = -0.5, e_3 = -1.5$.

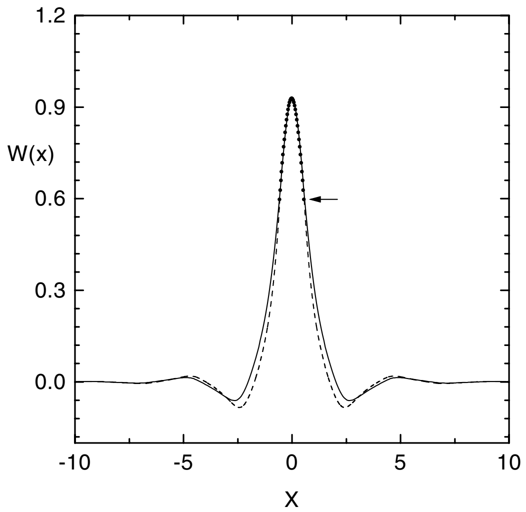

Figure 2. The WF associated to the lower band of the one-gap potential. The branching points of the elliptic curve are fixed as in figure 1. The amplitude of the function in the origin is $W(0) = 0.93$. The solid curve denotes the exact expression obtained from numerical calculations, the broken line corresponds to a part of the WF approximated by the asymptotic expansion, and the dotted line denotes the part obtained from the power expansion near the origin. The arrow shows the point where the two different analytical expansions are joined.

By comparing figure 3 with figure 2, we see that the discrepancy in the intermediate region is smaller for WF which are more localized. This can be understood from the fact that a faster decay of the function (see figures 4 and 5) allows the asymptotic expansion to work up to points that are very close to the origin. In figures 4 and 5, we show the asymptotic decay of the

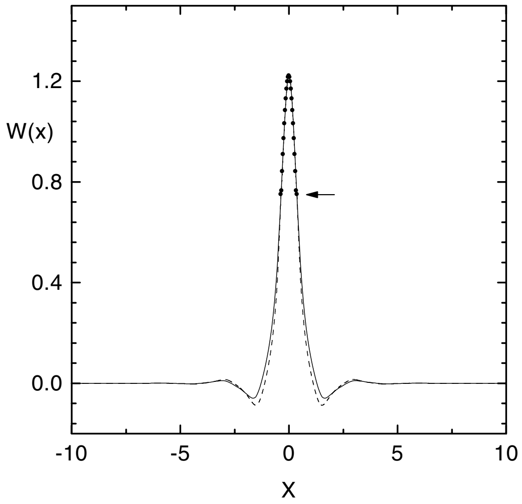

Figure 3. Same as in figure 2 but for a different set of parameters. The branching points of the elliptic curve are $e_1 = 6$, $e_2 = -2.0$, $e_3 = -4.0$. The value of the function in the origin is $W(0) = 1.22302$. The solid curve denotes the exact expression obtained from numerical calculations, the broken line corresponds to a part of the WF approximated by the asymptotic expansion, and the dotted line denotes the part obtained from the power expansion near the origin. The arrow shows the point where the two different analytical expansions are joined.

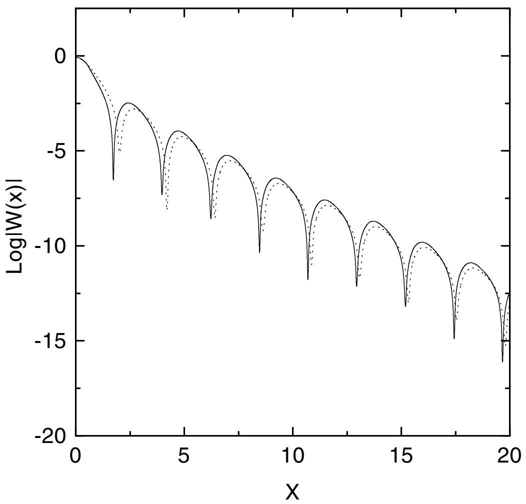

Figure 4. Asymptotic decay of the WF in figure 2 in semi-log scale. The solid curve represents our analytical approximation, while the dotted line is obtained from direct numerical calculations of the WF.

WF depicted in figures 2 and 3, respectively, from which we see that a stronger localization of the function corresponds to a faster asymptotic decay. The linear decay observed in the semi-log plots of these figures is fully consistent with the exponential decay of the WF of one-gap elliptic potentials predicted by our analysis.

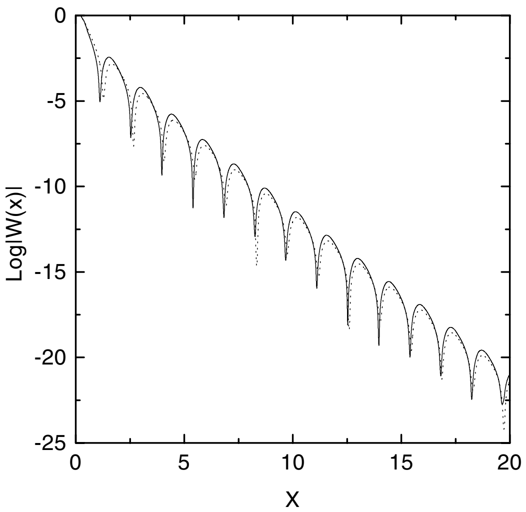

Figure 5. Asymptotic decay of the WF in figure 3 in semi-log scale. The solid curve represents our analytical approximation, while the dotted line is obtained from direct numerical calculations of the WF.

5. Conclusions

In this paper, we have investigated properties of the WF of the Schrödinger operator with one-gap potentials. As a result, we have derived the exact value for the amplitude of the functions in the origin, as well as an asymptotic expansion characterizing the decay of the function at large distances and a power series valid in the vicinity of the origin. Using these expansions, we have constructed approximate analytical expressions of the WF and have shown that they are in good agreement with the ones obtained from numerical results.

We remark that the approach developed here can be generalized to the case of finite-gap potentials of a more complicated type, like elliptic finite-gap potentials and general finite-gap potentials. We shall discuss these problems in a future publication and, in particular, in the forthcoming Proceedings of the Workshop 'Nonlinear waves: theory and experiment III', Gallipoli, 25 June–3 July 2004.

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