Wavelet Method for Computing Energy Band Diagram of Semiconductors

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Abstract
A wavelet expansion is applied for solving Schrödinger equation in order to compute band structure of an electronic crystal. In this paper we have used this method for finding band structure of one dimensional arbitrary potential. As discussed here, this algorithm could be easily applied to two- or three-dimensional arbitrary potentials. This paper is emphasizing on revealing the mathematical aspects of using wavelet expansion in computing electronic band structure. In order to find the full power of wavelets one needs to use this method in 2 or 3 dimension structures.

Keywords: Wavelet Method, Electronic Band Structure, Band Theory of Semiconductors

1. Introduction

It is of practical importance as well as of theoretical interest to know energy band structure of semiconductors so finding band structure with good accuracy and low computational cost is of interest. Equivalently any proposed method can be used for finding photonic band structure [1].The aim of this paper is to apply wavelet base method to the computation of band diagram in some standard cases of one dimensional models such as Krönig-Penney model. As it is known, the wavelet method provides much faster convergence rates than traditional methods [1] and flexibility for solving various equations such as Maxwell equation in time domain [2] and Navier-Stokes equations [3].

Nowadays there are various analytical methods for solving linear differential equation such as power series expansion method (Fröbenius) [4], plane wave expansion methods (PWE) [5] or numerical methods such as finite differences and finite elements [6]. The wavelet expansion method witch we will discus is similar to PWE method in some aspects. In plane wave method the solution of desired equation is expanded in sinusoidal bases but in wavelet method we simply replace sinusoidal bases by appropriate wavelet. Essential problems in PWE are: (1) Convergance problem due to Gibbs phenomena (2) Use of non-localized bases.

Wavelet expansion method benefits from (1) Faster convergence due to introducing a degree of freedom in choosing various types of wavelets (2) Unlike PWE they can describe discontinuities in an efficient way (3) Capability of multi resolution analysis due to localization in both frequency and spatial domains (4) Low computational cost (5) Final sparse matrix which simplifies numerical computation of eigenvalue.

In this paper we are emphasizing on revealing the mathematical aspects of using wavelet expansion in computing electronic band structure. A brief introduction to wavelet will be discussed in Section 2. Some useful wavelet properties are provided in Section 3. Next the algorithm used for computing band diagrams is described in Section 4. Results of band diagram calculation are presented in Section 5. More complex structures are mentioned in Section 6. Finally conclusion is added in Section 7.

2. Basics of Wavelets

The fundamental idea behind wavelets is to analyze according to scale. Indeed, the collections of wavelet together with scalet bases are form a complete set for square integrable function space.

From the vector space theory we know that any square integrable function can be expanded in following form [7,8]:

$$f(x)=\sum_{l\in Z}\alpha_l\varphi_{j_0,l}(x)+\sum_{l\in Z}\sum_{\substack{j\in Z\\ j\geq j_0}}\beta_{j,l}\psi_{j_0,l}(x), \quad (1)$$

where $\varphi(x)$ is called scalet which satisfies the equation

$$\varphi(x)=\sum_n h_n.\sqrt{2}\varphi(2x-n)$$

where the coefficients h_n are the impulse response values of the lowpass synthesis filter of a quadrature-mirror filter (QMF) filter bank and we have

$$\varphi_{j,l}(x)=2^{j/2}\varphi(2^j x-l)$$

Also $\psi(x)$ is called wavelet witch satisfies similar equation of $\varphi(x)$

$$\psi(x)=\sum_n g_n.\sqrt{2}\varphi(2x-n),$$

where $g_n=(-1)^n\bar{h}_{1-n}$ [8] and

$$\psi_{j,l}(x)=2^{j/2}\psi(2^j x-l).$$

In this paper for simplicity we use Daubechies (db5) wavelet (Fig. 1)

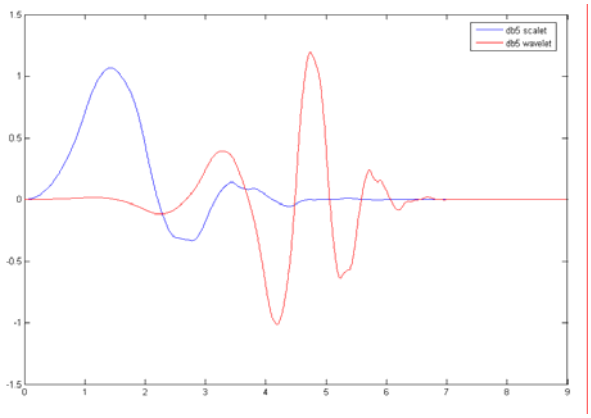

Fig. 1. Daubechies wavelet and scalet.

These wavelets have useful properties such as compact supported and orthonormality witch are discussed in section 3 in details.

An interesting property of wavelets is the number of vanishing moments defined by the greatest number *N* such that

$$\int_{-\infty}^{+\infty} x^s\psi(x)\,dx=0, \qquad for\ 0\le s<N.$$

As *N* increases it is expected that projection coefficient of a function on $\psi(x)$ decrease.

In our application, because of periodicity in crystal potential we must we must modify the conventional wavelets to periodic form. We can hence define periodic wavelets and scalets as follows:

$$\psi_{j,l}^{per}(x)=2^{j/2}\sum_{l\in Z}\psi\left(2^j(x+l)-n\right)$$

It is worthwhile that the above definition does not alter the (bi-)orthogonality properties.

3. Useful Wavelet Properties

An important property of wavelets witch we have used is (bi-)orthogonality. In the case of orthogonal wavelets the prime set is the same as dual set. But if we choose biorthogonal one we ought to define a dual set [9]. For simplicity we use orthogonal sets. Biorthogonal relation is defined as:

$$<\tilde{\varphi}_{j,l}\,|\,\varphi_{j,l'}>=\delta_{l'-l}$$

$$<\tilde{\psi}_{j,l}\,|\,\psi_{j',l'}>=\delta_{j'-j}\delta_{l'-l} \qquad l,l',j,j'\in Z$$

In the case of orthogonal wavelets the prime set is equal to dual set, that is:

$$\{\tilde{\psi},\tilde{\varphi}\}=\{\psi,\varphi\}$$

It is important to mention that if the wavelets are finite support then the following lemmas are hold:

Lemma I:

$$\int_{-\infty}^{+\infty}\psi_{j,l}(x).\psi'_{j,l}(x)dx=\frac{1}{2}\psi^2_{j,l}(x)\Big|_{-\infty}^{+\infty}=0$$

Lemma II:

$$\int_{-\infty}^{+\infty}\psi_{j,l}(x).\psi'_{j',l'}(x)dx=\psi_{j,l}(x).\psi_{j',l'}(x)\Big|_{-\infty}^{+\infty}$$

$$-\int_{-\infty}^{+\infty}\psi'_{j,l}(x).\psi_{j',l'}(x)dx$$

$$=-\int_{-\infty}^{+\infty}\psi'_{j,l}(x).\psi_{j',l'}(x)dx$$

Lemma III:

$$\int_{-\infty}^{+\infty}\psi_{j,l}(x).\psi''_{j',l'}(x)dx=\psi_{j,l}(x).\psi'_{j',l'}(x)\Big|_{-\infty}^{+\infty}$$

$$-\int_{-\infty}^{+\infty}\psi'_{j,l}(x).\psi'_{j',l'}(x)dx$$

$$=-\int_{-\infty}^{+\infty}\psi'_{j,l}(x).\psi'_{j',l'}(x)dx$$

In Section 4 we will use these lemmas to reduce the computational costs.

4. Algorithm

The problem at hand is to solve Schrödinger equation with the aid of wavelet expansion. The normalized Schrödinger equation reads:

$$-\frac{\partial^2 \Psi_K(x)}{\partial x^2} + V(x).\Psi_K(x) = E(K).\Psi_K(x) \quad (2)$$

where $E(K)$ is the energy and $\Psi_K(x)$ is the wave function of an electron with the wave number K in potential $V(x)$.

Using Bloch theorem and expanding wave functions $\Psi_K(x)$ in a truncated periodic wavelet basis we have:

$$\Psi(x) = \sum_n c_n B_n e^{jKx} \quad (3)$$

where B_n belongs to the following set:

$$B = \{\tilde{\varphi}_{j,l}, \tilde{\psi}_{j,l}\}$$

by substituting (3) in equation (2), after multiplying by B_m and integrating over a unit cell and we achieve:

$$-\sum\left(c_n \int B_m B^*_n\, dx + j\,2K\, c_n \int B_m B'_n dx\right) - K^2 c_m + \sum c_n \int B_m B_n V(x)\, dx = c_m E(K) \quad (4)$$

For reducing the computational cost and increasing precision we can use lemma 3 and reduce equation (4) to:

$$\sum\left(c_n \int B'_m B'_n dx + j\,2K\, c_n \int B_m B'_n dx\right) - K^2 c_m + \sum c_n \int B_m B_n V(x)\, dx = c_m E(K) \quad (5)$$

after transforming equation (5) into matrix form, it can be shown that:

$$A_{mn} = \int B'_m B'_n dx - j2K \int B_m B'_n dx + \int B_m B_n V(x) dx$$

noting lemma (1,2), the diagonal elements A_{nn} are purely real and the relation $A_{mn} = \overline{A}_{nm}$ holds true. Therefore we only need to compute the upper half elements of the matrix. As expected, the final matrix is Hermitian and the corresponding eigenvalue witch refers to energy become real. The final Matrix form is as follows:

$$\begin{bmatrix} A_{11} & & & \\ & A_{22} & B & \\ & & & \\ & \bar{B} & & A_{nn} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \\ c_n \end{bmatrix} = \left(E + K^2\right) \begin{bmatrix} c_1 \\ c_2 \\ \\ c_n \end{bmatrix}$$

In the final step one has to solve the matrix eigenvalue problem. There are several methods to do so in our case we are interested in few eigenvalue, that is the smallest ones. Hence we can use the classical iterative method [10].

As we see, in above matrix the derivative of basis appears in every single element, so the exact value of derivatives is of interest. Generally there is no analytical form for wavelets as well as their derivatives. For finding derivatives iteration methods are used. For initializing the iteration there are two choices: (1) Cascade algorithm (2) Exact algorithm [11].

In this paper, the exact algorithm is used to reduce the computational error. In order to expand this method for two- or three- dimensional potentials we only need to use 2D or 3D wavelets. It is easy to construct 2D wavelets with the aid of conventional wavelets only by applying tensor product [12].

5. Results

The algorithm just explained is programmed in Matlab software. The equation is solved for periodic step potential in figure 2 (conventional Krönig-Penney's model) with the aid of Daubechies 5 wavelet. The B set only contains 18 basis.

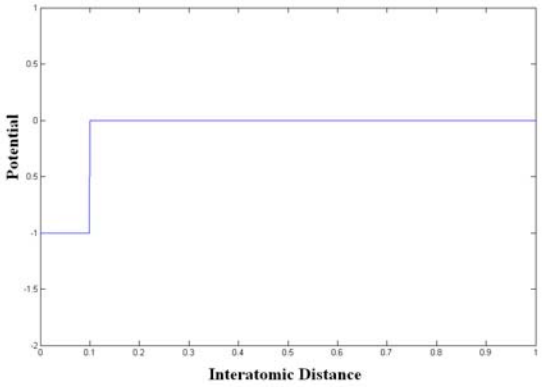

Fig. 2. One period of potential Note that the lattice constant is assumed to be 1 (*a*=1).

In Figure (3) the first four energy bands are drawn. Having used appropriate wavelets, results show that we can achieve high precision by using only a small number of bases and therefore lower computational cost could be achieved in comparison by plane wave method.

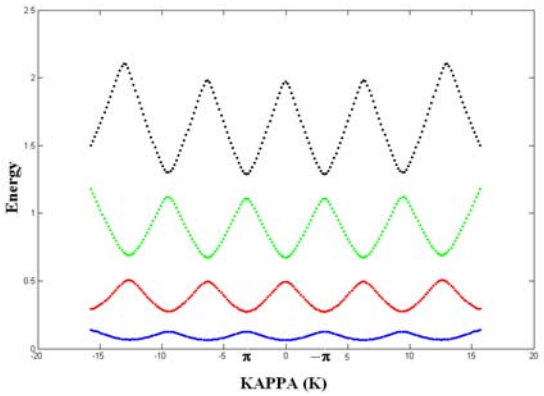

Fig. 3. Band diagram for Potential in figure 2. Note that this diagram is calculated for normalized equation.

It is noteworthy to point out that within a denormalization scaling constant, this result is in complete accordance with our other new method [14], which is based on the combination of Green's function and sampling techniques.

6. Conclusions

In this paper we have used wavelet expansion approach, for the first time, to find energy bands of semiconductor. We focused on demonstrating the algorithm as well as computational aspects. As we mentioned it is easy to develop this approach for two- or three-dimensional potentials. Also it seems that it is possible to solve Schrödinger eigenvalue problem with high accuracy while using only a small number of basis with the aid of suitable wavelets. This is the subject of our future research.

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