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COMMENT

Comment on 'Electronic minibands in complex basis superlattices: a numerically stable calculation'

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Abstract
Hsueh, Lin and Chen (HLC) (2007 *J. Phys.: Condens. Matter* **19** 266007) present a graph theory-based derivation of a stable method for determining the energy minibands of superlattices with an arbitrary number of layers per unit cell. Here it is shown that the above result is immediately derivable from the transfer matrix formalism by factoring out a single cosine function per layer.

HLC [1] deal with one-dimensional superlattices with N layers per unit cell. In their work they cite several papers on the subject and observe that most methods for calculating the band dispersions, such as the transfer matrix formalism [2, 3], suffer from numerical instabilities. Here it is shown that their results follow immediately from the transfer formalism. To show this, take the transfer matrix for the jth layer [4]

$$T_j(d_j) = \begin{pmatrix} \cos k_j d_j & \frac{\mathrm{i}\sin k_j d_j}{\alpha_j} \\ \mathrm{i}\alpha_j \sin k_j d_j & \cos k_j d_j \end{pmatrix} = \frac{1}{e_j}\begin{pmatrix} 1 & \frac{\mathrm{i}t_j}{\alpha_j} \\ \mathrm{i}\alpha_j t_j & 1 \end{pmatrix} \equiv \frac{1}{e_j} M_j\left(d_j\right), \quad (1)$$

where $\alpha_j = m_j^*/k_j$, $t_j = \tan k_j d_j$ and $e_j = \sec k_j d_j$, and a single cosine was factored out to produce the 2×2 matrix $M_j(d_j)$. For evanescent waves, k_j is imaginary, so that the sine and cosine functions turn into hyperbolic sines and cosines, functions that grow exponentially with layer width, hence the source of the numerical instabilities. HLC adopt the author's approach [4, 5] in seeking a formalism that employs tangents, since for evanescent solutions the hyperbolic tangents are bounded by ± 1.

Rather than using HLC's topological arguments to derive an eigenvalue condition with complicated recursion relations, it is much more transparent to use the eigenvalue condition for a periodic N-layer superlattice based on the transfer matrix formalism [4], i.e.

$$\left\| \frac{T_1(d_1)T_2(d_2)\cdots T_N(d_N)+T_N(-d_N)\cdots T_2(-d_2)T_1(-d_1)}{2} - \begin{pmatrix} \cos KL & 0 \\ 0 & \cos KL \end{pmatrix} \right\| = 0, \quad (2)$$

which in terms of the M matrices is

$$\left\| \frac{M_1(d_1)M_2(d_2)\cdots M_N(d_N)+M_N(-d_N)\cdots M_2(-d_2)M_1(-d_1)}{2(e_1 e_2\cdots e_N)} - \begin{pmatrix} \cos KL & 0 \\ 0 & \cos KL \end{pmatrix} \right\| = 0. \quad (3)$$

In view of the definition of the transfer matrix and its tangent form (1), the fact that the eigenvalue condition (3) can be written completely with tangents and secants is immediately obvious. Moreover, equation (3) provides a transparent algorithm (multiplication of 2×2 transfer matrices) for finding such an eigenvalue condition for any number of layers.

As an example, for two layers, from (3),

$$\left\| \frac{M_1\left(d_1\right) M_2\left(d_2\right) + M_2\left(-d_2\right) M_1\left(-d_1\right)}{2e_1 e_2} - \begin{pmatrix} \cos KL & 0 \\ 0 & \cos KL \end{pmatrix} \right\| = 0, \quad (4)$$

where, from (1),

$$M_1(d_1)\,M_2(d_2) = \begin{pmatrix} 1-\frac{\alpha_2}{\alpha_1}t_1t_2 & \mathrm{i}\left(\frac{t_1}{\alpha_1}+\frac{t_2}{\alpha_2}\right) \\ \mathrm{i}\,(\alpha_1 t_1+\alpha_2 t_2) & 1-\frac{\alpha_1}{\alpha_2}t_1t_2 \end{pmatrix}$$

$$\equiv \begin{pmatrix} A_2 & \mathrm{i}B_2 \\ \mathrm{i}C_2 & D_2 \end{pmatrix}, \tag{5}$$

where $A_2 = 1-\frac{\alpha_2}{\alpha_1}t_1t_2$, $B_2 = \frac{t_1}{\alpha_1}+\frac{t_2}{\alpha_2}$, $C_2 = \alpha_1 t_1+\alpha_2 t_2$, and $D_2 = 1-\frac{\alpha_1}{\alpha_2}t_1t_2$; at the same time,

$$M_2(-d_2)\,M_1(-d_1) = \begin{pmatrix} D_2 & -\mathrm{i}B_2 \\ -\mathrm{i}C_2 & A_2 \end{pmatrix}. \tag{6}$$

Using (5) and (6), equation (4) becomes $A_2 + D_2 - 2e_1e_2\cos KL = 0$, or

$$1-\frac{1}{2}\left(\frac{\alpha_2}{\alpha_1}+\frac{\alpha_1}{\alpha_2}\right)t_1t_2 - e_1e_2\cos KL = 0, \tag{7}$$

which is equation (17) of HLC.

For an arbitrary number of layers, one can proceed by induction. Assume that the forms (4) and (5) holds for $N-1$ layers, i.e. that

$$M_1(d_1)M_2(d_2)\cdots M_{N-1}(d_{N-1}) = \begin{pmatrix} A_{N-1} & \mathrm{i}B_{N-1} \\ \mathrm{i}C_{N-1} & D_{N-1} \end{pmatrix}, \tag{8}$$

$$M_N(-d_N)\cdots M_2(-d_2)M_1(-d_1) = \begin{pmatrix} D_{N-1} & -\mathrm{i}B_{N-1} \\ -\mathrm{i}C_{N-1} & A_{N-1} \end{pmatrix}, \tag{9}$$

and then show that these forms hold for N as well. First, for N layers, the product $[M_1(d_1)M_2(d_2)\cdots M_{N-1}(d_{N-1})]M_N(d_N)$ is given by

$$\begin{pmatrix} A_{N-1} & \mathrm{i}B_{N-1} \\ \mathrm{i}C_{N-1} & D_{N-1} \end{pmatrix}\begin{pmatrix} 1 & \frac{\mathrm{i}t_N}{\alpha_N} \\ \mathrm{i}\alpha_N t_N & 1 \end{pmatrix}$$

$$= \begin{pmatrix} A_{N-1}-B_{N-1}\alpha_N t_N & \mathrm{i}\left(B_{N-1}+A_{N-1}\frac{t_N}{\alpha_N}\right) \\ \mathrm{i}\,(C_{N-1}+D_{N-1}\alpha_N t_N) & D_{N-1}-C_{N-1}\frac{t_N}{\alpha_N} \end{pmatrix}$$

$$= \begin{pmatrix} A_N & \mathrm{i}B_N \\ \mathrm{i}C_N & D_N \end{pmatrix}, \tag{10}$$

where

$$A_N = A_{N-1} - B_{N-1}\alpha_N t_N, \tag{11a}$$

$$B_N = B_{N-1} + A_{N-1}\frac{t_N}{\alpha_N}, \tag{11b}$$

$$C_N = C_{N-1} + D_{N-1}\alpha_N t_N, \tag{11c}$$

$$D_N = D_{N-1} - C_{N-1}\frac{t_N}{\alpha_N}; \tag{11d}$$

then the product $M_N(-d_N)[M_{N-1}(-d_{N-1})\cdots M_2(-d_2)M_1(-d_1)]$ is found to be

$$\begin{pmatrix} 1 & -\frac{\mathrm{i}t_N}{\alpha_N} \\ -\mathrm{i}\alpha_N t_N & 1 \end{pmatrix}\begin{pmatrix} D_{N-1} & -\mathrm{i}B_{N-1} \\ -\mathrm{i}C_{N-1} & A_{N-1} \end{pmatrix}$$

$$= \begin{pmatrix} D_{N-1}-C_{N-1}\frac{t_N}{\alpha_N} & -\mathrm{i}\left(B_{N-1}+A_{N-1}\frac{t_N}{\alpha_N}\right) \\ -\mathrm{i}\,(C_{N-1}+D_{N-1}\alpha_N t_N) & A_{N-1}-B_{N-1}\alpha_N t_N \end{pmatrix} \tag{12}$$

which indeed is equal to $\begin{pmatrix} D_N & -\mathrm{i}B_N \\ -\mathrm{i}C_N & A_N \end{pmatrix}$. Having proved the theorem, equations (11*a*)–(11*d*) become the recursion relations that replace the complex formulae (8)–(12) of HLC. Altogether, for any N, from equation (3)

$$\frac{A_N + D_N}{2} - (e_1e_2\cdots e_N)\cos KL = 0, \tag{13}$$

where, through equations (11*a*)–(11*d*), A_N and B_N are expressed in terms of tangents only and are simpler to code than the equations in HLC. Equation (13) has the form of equation (14) of HLC and involves only tangents and secants. Tangent-only forms can be found in the author's work [4, 5].

In conclusion, the tangent and secant form for the N-layer Kronig–Penney model is immediately and simply derivable from the transfer matrix formalism.

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