Reply to comment on 'Electronic minibands in complex basis superlattices: a numerically stable calculation'

# REPLY

# Reply to comment on 'Electronic minibands in complex basis superlattices: a numerically stable calculation'

## W J Hsueh and F J Yang

Department of Engineering Science, National Taiwan University, 1, Section 4, Roosevelt Road, Taipei 10660, Taiwan

E-mail: hsuehwj@ntu.edu.tw

**Abstract**
In the comment by Szmulowicz (2008 *J. Phys.: Condens. Matter* **20** 088001) on our recent paper (Hsueh *et al* 2007 *J. Phys.: Condens. Matter* **19** 266007), the author claimed that the formula in our work is immediately derivable from the transfer matrix formalism using only the factoring out cosine function. In the response, we demonstrate that the formula presented in our original paper is not the same as that proposed in the comment. It is difficult to obtain our formula by the method given in the comment. We also respond to some other criticisms of the original work raised in the comment.

Szmulowicz presented an alternative transfer matrix method to calculate the miniband structure in superlattices in the comment [1] on our published paper (Hsueh *et al* 2007 *J. Phys.: Condens. Matter* **19** 266007, here called HLC) [2]. He claims in the abstract of the comment that 'the above result [the HLC formula] is immediately derivable from the transfer matrix formalism by factoring out a single cosine function per layer'. We do not agree with this statement. In the comment, the eigenvalue condition is expressed by a new global transfer matrix $M$ and a secant term, $e_1 e_2 \ldots e_N$, as given in equations (3) and (13). Although both formulae for the dispersion relations presented by HLC and that by the Szmulowicz method consist of tangents and secants, it is clear that any one of equations (3) and (13) in the comment are not the same as any one of our equations, that is, equations (14) or (15) of our original paper.

In the comment, the dispersion equation for a two-layer basis superlattice derived by our paper, given in equation (17), is derived by the transfer matrix method. However, for a number of layers in each cell greater than three, it is not possible to derive the dispersion equation with the HLC expression in the comment using the Szmulowicz method. Moreover, the general form of the dispersion equation for the $N$-layer basis as given in formulae (14) or (15) of our paper has not been derived in the comment. It is unreasonable

to infer that the formulae presented in the original work are immediately derivable from the transfer matrix method only according to a two-layer case.

To see the difference between the HLC and Szmulowicz methods, the $N$-layer basis superlattice studied in the example of the original paper [2] is also examined by the method presented in the comment. In the example, for each period of the superlattice, the concentration of each odd layer is 0 and that of each even layer is 0.5. The width of each layer in each period is $d_n = 2(1 + \frac{n}{N})nm$. Figure 1 shows that the upper and lower bounds defined respectively by the maximum and the minimum absolute values of each element of the global transfer matrix $M$ given in the comment are calculated versus $N$ changeable from 2 to 80. We find that the upper bounds of the elements $M_{11}$ and $M_{22}$ of the global transfer matrix given in the comment enlarge exponentially from $10^3$ to $10^{42}$ and from $10^3$ to $10^{40}$, respectively, when $N$ increases from 2 to 80. Moreover, the upper bounds of other elements and the secant term, $e_1 e_2 \ldots e_N$, also enlarge exponentially for increasing $N$. The lower bound of the secant term, $e_1 e_2 \ldots e_N$, decreases exponentially from $10^{-1}$ to $10^{-49}$ for $N$ increasing from 2 to 80. According to the numerical results, we see that the method presented by Szmulowicz may not be numerically stable, even when the cosine function for each layer is factored out. However, in our paper, the maximum absolute values
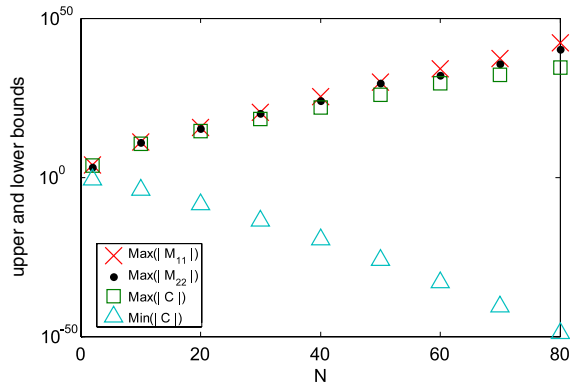
**Figure 1.** The upper and lower bounds in the calculation of band structure of an $N$-layer basis superlattice by the method presented in the comment by Szmulowicz. The structure and the parameters of the superlattice are defined in the original work and given by $d_n = 2(1 + \frac{n}{N})$ nm, $x_1 = x_3 = \cdots = x_{N-1} = 0$, $x_2 = x_4 = \cdots = x_N = 0.5$. The function $C$ is defined by the factored terms $C = e_1 e_2 \ldots e_N$. The upper and lower bounds of function $C$ are denoted by Max($|C|$) and Min($|C|$).

(This figure is in colour only in the electronic version)

of each term used in our paper do not enlarge with increased $N$. From the numerical results, this indicates that the method presented in the original work differs from that in the comment.

In the comment, the author also states 'Rather than using HLC's topological arguments to derive an eigenvalue condition with complicated recursion relations, …'. The author of the comment may misunderstand the expression of our formulae. The expressions for the functions $S^{p,q}$, $f$, $g$ and $h$, given in equations (9)–(12) of the original paper are finite series forms, which are analytical and closed-form rather than recursive relations.

The author of the comment claims 'For evanescent waves, …, hence the source of the numerical instability. 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 $\pm 1$'. However, according to the results shown in figure 1, we see that this claim is not completely correct. Numerical stability in the calculation by our method is not only induced by the tangents formulation but also by the expression of the formulae.

In summary, with the results presented, we find that some criticisms in the comment on the original work are unreasonable. The formula for the dispersion equation in our paper is not the same as that proposed in the comment. It is difficult to obtain our formula by the transfer matrix formalism only using the factoring out cosine function. Moreover, the expressions of the dispersion equations presented in the original work are finite series forms rather than recursive relations. In the original work, numerical stability in the calculation is not only induced by the tangents formulation but also by the expression of the formulae.

## Acknowledgment

## References

[1] Szmulowicz F 2008 *J. Phys.: Condens. Matter* **20** 088001
[2] Hsueh W J, Lin J C and Chen H C 2007 *J. Phys.: Condens. Matter* **19** 266007