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Elimination of spurious solutions from $k\cdot p$ theory with Fourier transform technique and Burt-Foreman operator ordering

Qiuji Zhao,¹ Ting Mei,^{2,a)} and Dao Hua Zhang¹

¹School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

²Institute of Optoelectronic Materials and Technology, South China Normal University, Guangzhou 510631, China

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To eliminate spurious solutions in the multiple-band $k\cdot p$ theory, we developed the Fourier transform-based $k\cdot p$ approach through combining the Fourier transform technique with Burt-Foreman operator ordering. The performance is perfect for the six-band $k\cdot p$ calculation, and the spurious solutions in the conduction band met in the eight-band calculation can also be easily screened away in the inborn cut-off step in FTM, i.e., choosing a proper order of Fourier truncation. Truncating high-order terms of Fourier coefficients of the envelope function prevents the occurrence of a wild-spreading spectrum of the Fourier expansion coefficients, which can be taken as the signature of spurious solutions. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.3689821>]

I. INTRODUCTION

In contrast to the computationally intensive *ab initio* and atomistic models, multiband effective mass approximation (EMA) in the envelope function representation has served as an important and powerful tool to solve the electronic structures of heterostructures specifically. Unfortunately, appearance of spurious solutions is one of the main problems of EMA $k\cdot p$ model, especially for the case with large wave vectors. The so called wing-band (evanescent) solutions^{1–4} do not contribute to effective-mass wave functions and thus the elimination of spurious solutions has been seldom discussed, whereas, the oscillatory solutions^{5–7} are indeed troublesome and the elimination of oscillatory solutions in the $k\cdot p$ theory is still a hot topic.

The origin of oscillatory spurious solutions is still controversial and interpreted as multifarious reasons. It has been stated that the perturbative nature and the incomplete set of basis functions of the $k\cdot p$ theory cause the nonmonotonic behavior of the conduction band with increasing k due to the coupling with valence bands.^{6–8} Burt⁹ and Foreman^{10,11} ascribed the reason to the adoption of the improper symmetrized operator ordering, which is not a necessary condition for the multiband Hamiltonian for heterostructures to be Hermitian. Recently, Veprek *et al.*^{12,13} demonstrated that necessary fitting of bulk material parameters to experimental data for heterostructure calculations leads to the difficulty to satisfy the ellipticity of the differential operator. Lassen *et al.*¹⁴ stated that envelope functions satisfying the boundary condition would have components outside the first Brillouin zone and thus present the spurious solutions. And even the finite difference scheme may also induce spurious solutions.¹⁵

Though no completely effective way has been put forward to resist oscillatory solutions, three general methods have been proposed to eliminate spurious solutions in some extent. The

first is modification of the Hamiltonian by discarding the coupling of conduction band and valence band,¹⁶ by adding a term proportional to ∇^4 to the Hamiltonian,⁷ or by introducing an off-diagonal k^2 term.¹⁶ This method has not been widely adopted due to the cumbersome implement and subsequent fixes compromising the initial idea of the effective-mass model. The second is revision of the improper symmetrized operator ordering to the Burt-Foreman (BF) operator ordering. Spurious solutions in the conduction band is further eliminated either by setting the coefficient of k^2 in the conduction-band (CB) matrix element to zero (i.e., $A_c = 0$) and fitting the CB mass with momentum matrix element P (i.e., optical matrix element E_p as $E_p = P^2 2m_0/\hbar^2$),¹¹ or by reducing E_p to cater the ellipticity of the differential operator.¹² This method is verified to be effective to eliminate spurious solutions in the valence band (VB)^{10–13,17} except for residual spurious solutions in the CB. The price is that other effective mass parameters also change simultaneously, and there is still uncertainty about which basis is chosen to determine the literature parameters though A_c and P (E_p) can be set to arbitrary values with a change of Bloch basis.^{12,18} The third is the cut-off method, i.e., discarding the large- k solutions as unphysical, which is very simple and robust for any kind of spurious solutions and thus is widely implemented.^{1,3,8,14,19,20} Consequently, it should be more effective and powerful to combine the cut-off method with BF operator ordering to tackle the problem of spurious solutions in the $k\cdot p$ theory, which is main topic of this work.

In this article, after recapturing the theorem of Fourier transform $k\cdot p$ method (FTM) adopting symmetrized operator ordering (denoted as SYM FTM) in Refs. 20 and 21, we develop the refined FTM with BF operator ordering (denoted as BF FTM). We employ several zinc blende (ZB) and wurtzite (WZ) quantum structure examples including quantum wells (QWs) and quantum wires (QWRs) to demonstrate that merging the cut-off method and BF operator ordering is really a powerful approach to clean up spurious solutions in both CB and VB. Screening of spurious solutions via Fourier

^{a)}Author to whom correspondence should be addressed. Electronic mail: ting.mei@iee.org.

truncation without any special treatment of interfaces and the cause of spurious solutions under a large Fourier truncation order are detailed as well.

II. FTM WITH BURT-FOREMAN OPERATOR ORDERING

With the following basis,

$$|S \uparrow\rangle, |X \uparrow\rangle, |Y \uparrow\rangle, |Z \uparrow\rangle, |S \downarrow\rangle, |X \downarrow\rangle, |Y \downarrow\rangle, |Z \downarrow\rangle, \quad (1)$$

$$\begin{pmatrix} kA_c k + E_c & \frac{i}{2}(v_1 k_x + k_x v_2) & \frac{i}{2}(v_1 k_y + k_y v_2) & \frac{i}{2}(v_1 k_z + k_z v_2) \\ -\frac{i}{2}(v_2 k_x + k_x v_1) & H_{XX} + E_v - \frac{\Delta}{3} & k_x \tilde{N}_+ k_y + k_y \tilde{N}_- k_x & k_x \tilde{N}_+ k_z + k_z \tilde{N}_- k_x \\ -\frac{i}{2}(v_2 k_y + k_y v_1) & k_y \tilde{N}_+ k_x + k_x \tilde{N}_- k_y & H_{YY} + E_v - \frac{\Delta}{3} & k_y \tilde{N}_+ k_z + k_z \tilde{N}_- k_y \\ -\frac{i}{2}(v_2 k_z + k_z v_1) & k_z \tilde{N}_+ k_x + k_x \tilde{N}_- k_z & k_z \tilde{N}_+ k_y + k_y \tilde{N}_- k_z & H_{ZZ} + E_v - \frac{\Delta}{3} \end{pmatrix}, \quad (3)$$

where the inversion symmetry parameter B is equal to zero,^{23,24} and the split of momentum matrix element P in the coupling between CB and VB is $v_1 = 2P$ and $v_2 = P$, respectively.¹⁷ The component comprising A_c and E_c is the scalar description of CB and the typical diagonal component for VB is

$$H_{XX} = k_x \tilde{L}' k_x + k_y \tilde{M} k_y + k_z \tilde{M} k_z. \quad (4)$$

The other diagonal elements for VB are given by cyclic permutation of x , y , and z . $\tilde{N}_+$ and $\tilde{N}_-$ are the split of $\tilde{N}$ with the relationship,

$$\tilde{N}' = \tilde{N}_+ + \tilde{N}_-, \quad (5)$$

where $\tilde{N}_-$ is estimated as

$$\tilde{N}_- = M - \frac{\hbar^2}{2m_0}. \quad (6)$$

As $v_1 = v_2 = P$ and $\tilde{N}_+ = \tilde{N}_- = \tilde{N}'/2$, the BF operator ordering becomes the symmetrized operator ordering. E_c and E_v represent the conduction and valence band edges, respectively; Δ is the spin-orbit splitting; and $\tilde{L}'$, $\tilde{M}$, and $\tilde{N}'$ are renormalized Kane parameters and expressed with modified Luttinger parameters using,¹²

$$\begin{aligned} \tilde{L}' &= -\frac{\hbar^2}{2m_0}(\tilde{\gamma}_1 + 4\tilde{\gamma}_2), \\ \tilde{M} &= -\frac{\hbar^2}{2m_0}(\tilde{\gamma}_1 - 2\tilde{\gamma}_2), \\ \tilde{N}' &= -\frac{\hbar^2}{2m_0}6\tilde{\gamma}_3. \end{aligned} \quad (7)$$

the eight-band $k \cdot p$ Hamiltonian for the ZB bulk crystal is written as,²²

$$H = \begin{pmatrix} H_4 & \mathbf{0} \\ \mathbf{0} & H_4 \end{pmatrix} + H_{so}, \quad (2)$$

where H_{so} is spin-orbit Hamiltonian given in Eq. (4b) of Ref. 22. As a direct consequence of BF operator ordering, the block of H_4 is expressed as,^{10–12,17}

In the eight-band computation, modified Luttinger parameters $\tilde{\gamma}_i$ are subtracted Luttinger parameters γ_i with,²⁵

$$\begin{aligned} \tilde{\gamma}_1 &= \gamma_1 - \frac{E_p}{3E_g}, \\ \tilde{\gamma}_2 &= \gamma_2 - \frac{E_p}{3E_g}, \\ \tilde{\gamma}_3 &= \gamma_3 - \frac{E_p}{6E_g}, \end{aligned} \quad (8)$$

where E_g represents the bandgap.

The renormalized CB effective mass parameter A_c is a tunable parameter and the following expression is adopted in this article,

$$A_c = \frac{\hbar^2}{2m_c^*} - \frac{2P^2}{3E_g} - \frac{P^2}{3(E_g + \Delta)}. \quad (9)$$

The bulk Hamiltonian matrix is applicable to heterostructures as $k_i = -\nabla_i$. With BF operator ordering, the envelope function for the heterostructures is solved by the following eigen equation,

$$\mathbf{H}(\mathbf{r}; \mathbf{k}) \mathbf{F}(\mathbf{r}) = E(\mathbf{k}) \mathbf{F}(\mathbf{r}), \quad (10)$$

where k_i is replaced with $\hat{k}_i$ and Hamiltonian is

$$\mathbf{H} = \sum_{i,j} \hat{k}_i H_{ij}^{(2)}(\mathbf{r}) \hat{k}_j + \sum_i \left[H_{i,L}^{(1)}(\mathbf{r}) \hat{k}_i + \hat{k}_i H_{i,R}^{(1)}(\mathbf{r}) \right] + H^{(0)}(\mathbf{r}). \quad (11)$$

The envelope function can be expressed in plane-wave expansion along the quantum confined direction(s),^{20,21}

$$\mathbf{F}(\mathbf{r}) = \begin{cases} e^{ik_x x + ik_y y + ik_z z} \frac{1}{\sqrt{d_z}} \sum_{n_z} \mathbf{c}_{n_z} e^{in_z K_z z} & \text{for QW} \\ e^{ik_x x + ik_y y + ik_z z} \frac{1}{\sqrt{d_x d_y}} \sum_{n_x} \sum_{n_y} \mathbf{c}_{n_x n_y} e^{i(n_x K_x x + n_y K_y y)} & \text{for QWR} \end{cases}, \quad (12)$$

where d_α denotes the periodicity, $\kappa_\alpha = 2\pi/d_\alpha$, $-(\kappa_\alpha/2) < k_\alpha < \kappa_\alpha/2$, α is the suffix representing directions in Cartesian coordination system, i.e., x, y, z , and $\mathbf{c}_n = [c_1, c_2, \dots, c_8]^T$. If there are N superlattice periods, the Born-Von Karman cyclic boundary condition²⁶ gives

$$k_\alpha = \frac{2\pi j}{Nd_\alpha}, 0 \leq j \leq N. \quad (13)$$

Equation (10) can be completely handled in Fourier domain with Fourier series of $H(\mathbf{r}; \mathbf{k})$.^{20,21} This approach takes advantage of orthogonality of complex componential functions to evade the cumbersome integral calculation and presents the equation for eigen-problem as,

$$[\mathbf{M}_{um,vn}][\mathbf{c}_{vn}] = E[\mathbf{c}_{vn}], \quad (14)$$

where the Hamiltonian matrix in Fourier domain, $\mathbf{M}_{um,vn}$, is expressed with Fourier series $\tilde{H}^{(\alpha\beta)}$, $\tilde{H}_L^{(\alpha)}$, $\tilde{H}_R^{(\alpha)}$ and $\tilde{H}^{(0)}$ of the k - p Hamiltonian in the real space,

$$\begin{aligned} \mathbf{M}_{um,vn} = & \sum_{\alpha,\beta} \tilde{H}_{uv,q_i=m_i-n_i}^{(\alpha\beta)} (k_\alpha + m_\alpha \kappa_\alpha) (k_\beta + n_\beta \kappa_\beta) \\ & + \sum_{\alpha} \tilde{H}_{uv,q_i=m_i-n_i,L}^{(\alpha)} (k_\alpha + n_\alpha \kappa_\alpha) \\ & + \sum_{\alpha} \tilde{H}_{uv,q_i=m_i-n_i,R}^{(\alpha)} (k_\alpha + m_\alpha \kappa_\alpha) + \tilde{H}_{uv,q_i=m_i-n_i}^{(0)}, \end{aligned} \quad (15)$$

where β is also a suffix similar to α . The derivation is presented with QW as an example in the Appendix.

The dimension of the Fourier-domain Hamiltonian $\mathbf{M}$ is only determined by the order of the Fourier frequencies of $\mathbf{H}$. An arbitrary heterostructure may result in an infinite dimension of $\mathbf{M}$, but practically, the Fourier spectrum has negligible magnitudes at high frequencies and thus can be truncated. If terms up to N th order in Fourier series are retained in the wavefunction, i.e., $n_\alpha, m_\alpha = -N_\alpha, \dots, 0, \dots, N_\alpha$, the Fourier series terms of $\mathbf{H}$ will be reserved up to the $2N_\alpha^{\text{th}}$ order, i.e., $q_\alpha = m_\alpha - n_\alpha = -2N_\alpha, \dots, 0, \dots, 2N_\alpha$ ($N_\alpha < n_\alpha/4$ is used to serve the demand of Nyquist sampling theorem). Therefore, the dimension of $\mathbf{M}$ is only determined by the truncation frequencies N_α , i.e., $V \prod_{\alpha} (2N_\alpha + 1) \times V \prod_{\alpha} (2N_\alpha + 1)$, where V is the number of bands involved in

the calculation. Of course, splitting the first order Hamiltonian into two parts results in larger computation volume for BF operator ordering, compared with symmetrized operator ordering.

The plane-wave expansion is a commonly adopted approach for the k - p method. The wave basis cut-off is inborn with plane-wave expansion based methods. In contrast to most works that solved eigen-problems in real space, our approach handles the equation in the Fourier domain, via Fourier transforming the spatial-domain Hamiltonian matrix to the Fourier domain using the orthogonal feature of the basis functions of the Fourier representation. Since high-order Fourier components of $\mathbf{H}$ are truncated in our computation, "Fourier truncation" in this circumstance has two aspects: truncation of high-order Fourier components of $\mathbf{H}$ and in

parallel with the wave basis cut-off for the plane-wave expansion, which is far more than the simple wave-basis cut-off investigated in previous reports.

The formulation of FTM with BF operator ordering is illustrated with ZB crystals. However, Eq. (15) is also applicable to WZ crystals, even for Hamiltonian written in other bases. Though strain effect is not discussed in this paper, strain Hamiltonian with BF operator ordering in the momentum space can be derived via applying the above procedure on Eq. (25) in Ref. 23.

III. RESULTS AND DISCUSSIONS

Comparison between results of symmetrized operator ordering and BF operator ordering has been carried out with finite element method (FEM) by Veprek *et al.*¹² They also reported that spurious solutions turn up in the usually unaffected six-band k - p model and surmised that these unwanted spurious solutions cause the rare adoption of FEM, in contrast to the widely used FDM and plane-wave expansions. Consequently, it is necessary to see whether the spurious solutions turn up in the six-band k - p model realized by the very different FTM based on plane-wave expansion of spatial Hamiltonian. Furthermore, the order of Fourier truncation N_{tr} is a vital factor in the FTM computation for eight-band k - p Hamiltonian, as N_{tr} not only controls accuracy of computation^{20,21} but also can be used to screen away spurious solutions.²⁰ We therefore plot the first four VB band structures of a 50 Å InAs/GaAs ZB QW under various N_{tr} in Fig. 1, where the computation is carried out using both the six-band SYM FTM [Fig. 1(a)] and the six-band BF FTM [Fig. 1(b)], and the material parameters follow Table I in Ref. 12. It can be seen in Fig. 1(a) that the solutions are not stable for varying N_{tr} and spurious solutions arise at the large- k , in accompany with oscillatory wave functions (not shown here). In contrast, all solutions in Fig. 1(b) obtained with BF operator ordering are consistent as N_{tr} varies from 20 to 127. As shown by these results in the six-band k - p calculation for QWs, BF FTM performs well for rejecting spurious solutions without any control of N_{tr} , however, there is no convergence among the solutions of SYM FTM for varying N_{tr} . The existence of such unwonted spurious solutions in both FTM and FEM may suggest that these spurious solutions are not subject to the numerical method, but to the envelope equations.

As detailed in Sec. II, the most significant feature of BF operator ordering is the nonuniform splitting of momentum matrix P and renormalized Kane parameter $\tilde{N}'$ in Eq. (3). Nonuniform splitting of P acts on the coupling between CB and VB, while nonuniform splitting of $\tilde{N}'$ on the coupling in VB. However, there is no such a similar nonuniform splitting of A_c for the CB component. Therefore, it is easily predicted that BF operator ordering would not make the energy states in CB much different from those obtained using symmetrized operator ordering, especially for the QW heterostructure with quantization occurring in only one dimension. We therefore employ the above 50 Å InAs/GaAs ZB QW again and compare the results of eight-band SYM FTM and eight-band BF FTM, where the material parameters follow Table III with no reduced E_p in Ref. 12. The fact is exactly that CB

FIG. 1. (Color online) Energy band structures of an InAs/GaAs QW obtained using the six-band Hamiltonian matrix for a series of Fourier truncation N_{tr} : (a) with symmetrized operator ordering (denoted as SYM FTM) and (b) with BF operator ordering (denoted as BF FTM).

energy dispersion in SYM FTM solution is totally in consistency with that BF FTM solution regardless of the choice of N_{tr} , even the same for the VB energy dispersion. This phenomenon is very similar to that reported by Veprek *et al.*¹² Figure 2 just shows the eight-band BF FTM solutions for $N_{tr} = 20, 106, 107, 127$. As N_{tr} varies from 20 to 127, no spurious solutions appears in VB, while spurious solutions

FIG. 2. (Color online) Energy band structures of an InAs/GaAs QW obtained using the eight-band BF FTM for a series of orders of Fourier truncation N_{tr} .

emerge in CB since $N_{tr} = 107$. That is to say that spurious solutions in the eight-band calculation for heterostructures with 1D quantization tends to locate in CB band, and BF operator ordering fails to resist them, which may be possibly caused by the coupling between CB and VB. In such situation, it depends on the choice of N_{tr} , i.e., cut-off high order Fourier frequencies, to makes up the deficiency of BF operator ordering in avoiding the spurious solution issue for the eight-band $k \cdot p$ computation for QWs. The most significant merit of such cut-off in FTM is that there is no requirement for manipulating material parameters or setting specific boundary conditions as done in Ref. 11.

The energy eigenvalues of a 50 Å InAs/GaAs QW are calculated using eight-band BF FTM and material parameters from Table III with no reduced E_p in Ref. 12. Obtained energies locating at the center of Brillouin zone ($k_t = 0$) and at the edge of Brillouin zone ($k_t = 0.2$) are then plotted versus the order of Fourier truncation (N_{tr}) for different numbers of mesh points (N) in Figs. 3(a) and 3(b), respectively, showing that spurious solutions turn up earlier for greater k_t in CB while present only for nonzero k_t in VB. This observation agrees to the fact that spurious solutions are prone to occur at large k region. The plots also show that it is N_{tr} that controls the occurrence of spurious solutions in FTM, not the step size of discretization as in FDM.¹⁵ The cut-off method

FIG. 3. (Color online) Energy band diagram of a 50 Å InAs/GaAs QW calculated using BF FTM varies with different orders of Fourier truncation (N_{tr}) and different mesh points (N): (a) energy states locate at center of Brillouin zone ($k_t = 0$), and (b) energy states locates at the edge of Brillouin zone ($k_t = 0.2$). The two dashed lines indicated the forbidden band region.

trades off the computation accuracy for controlling spurious solutions, but in practice sufficient accuracy has been achieved before spurious solutions take place. Therefore, the range for selecting N_{tr} may be quite large. As a rule of thumb, smaller N_{tr} is demanded to resist spurious solutions for heterostructures with sharp interfaces, i.e., sharp geometry or drastic difference of material parameters.

Lassen *et al.*¹⁴ split the set of Schrödinger Hamiltonian in the k -space $\hat{H}$ into two parts (the main part $\hat{H}_{nn'}^0$ and the rest part $\hat{H}_{nn'}^1$) using a unitary operator which blocks diagonalizes $\hat{H}$, and verified that spurious solutions can be controlled as $\hat{H}_{nn'}^1$ is indeed small compared to $\hat{H}_{nn'}^0$ via adopting small k , i.e., to cutoff the large k components. They also

have stated that the failure to restrict Fourier expansion coefficient $\mathbf{c}_n$ in Eq. (12) to small k components would lead to the appearance of spurious solutions. In our FTM, hiring large N_{tr} may also possibly cause the wild spread of Fourier expansion coefficient $\mathbf{c}_n$, upon which spurious solutions take place. In Fig. 4, we therefore plot the electron ground state's CB component of the Fourier expansion coefficients $\mathbf{c}_n$ for the solutions shown in Fig. 3(a) at $N_{tr}=40$, $N_{tr}=115$ and $N_{tr}=127$. The first Brillouin zone is marked within two dashed lines. Fourier series $\mathbf{c}_n$ of envelope functions is confined well in the first Brillouin zone at $N_{tr}=40$, but falls out of the Brillouin zone since $N_{tr}=115$, which is exactly the point where the electron ground-state eigen energy starts to diverge in Fig. 3(a). Hence, the wild-spreading spectrum of the Fourier expansion coefficient $\mathbf{c}_n$ can be taken as the signature of spurious solutions. One point need to mention is that the divergent energy may also vibrate to be the same value as that associated with smaller N_{tr} , therefore it seems that energies at $N_{tr}=127$ in Fig. 2 are not spurious solutions.

This is further examined in the QWR case. The energy band structure of a wurtzite $18\text{ Å} \times 18\text{ Å}$ square GaN/AlN QWR is obtained by the six-band k - p calculation with both SYM and BF orderings, as shown in Fig. 5. Material parameters used in the computation are adopted from Ref. 27. Fig. 5 is similar to Fig. 1, the solutions by BF ordering are very

FIG. 4. (Color online) Fourier series $\mathbf{c}_n$ of envelope functions particular to the CB ground state of a 50 Å InAs/GaAs QW with orders of Fourier truncation (a) $N_{tr}=40$, (b) $N_{tr}=115$, and (c) $N_{tr}=127$. The computation is done with BF FTM at $k_t=0$ and the region composed by two dashed lines indicates the Brillouin zone.

FIG. 5. (Color online) Energy band structures of an $18\text{ Å} \times 18\text{ Å}$ square GaN/AlN QWR obtained using the six-band Hamiltonian matrix for a series of orders of Fourier truncation N_{tr} : (a) with symmetrized operator ordering (SYM FTM) and (b) with BF operator ordering (BF FTM).

FIG. 6. (Color online) Probability density function of an $18 \text{ \AA} \times 18 \text{ \AA}$ square GaN/AlN QWR with (a) $N_{tr}=10$ and (b) $N_{tr}=11$ and the corresponding Fourier series $\mathbf{c}_n$ of the envelope function particular to VB ground state with (c) $N_{tr}=10$ and (d) $N_{tr}=11$. The computation is done with SYM FTM at $k_i=0$ and dashed boxes in (c) and (d) indicated first Brillouin zones.

stable, while in calculation with SYM ordering spurious solutions quickly turn up with increasing k and appear even at $k_i=0$. Only at the very small N_{tr} ($N_{tr}=5$), the energy dispersion shows similarity to that obtained by BF ordering in Fig. 5(b), and can be considered as true solution, even though the accuracy is poor at a small truncation order. The probability density functions and the Fourier series $\mathbf{c}_n$ of envelop functions of the ground state obtained using SYM ordering are plotted in Fig. 6 for $N_{tr}=10$ and at $N_{tr}=11$. The two first Brillouin zones are marked within dashed box. Unlike that in Fig. 6(a), the probability density function in Fig. 6(b) is located at the corner of QWR, indicating this solution is non-physical. Fourier series $\mathbf{c}_n$ of envelope functions at $N_{tr}=11$ shown in Fig. 6(d) falls out of the first Brillouin zone. In contrast, the one corresponding to the solution with physical meaning in Fig. 6(c) falls inside the first Brillouin zone. Recalling the case of QW computed with BF FTM in Fig. 4, we can further confirm that large N_{tr} may fail to confine Fourier series $\mathbf{c}_n$ of envelope function in the small k -region and thus allow spurious solutions, no matter what kind of heterostructures and what kind of operator ordering.

IV. CONCLUSIONS

BF operator ordering has been incorporated into FTM to boost the capability of tackling spurious solutions in the multi-band $k \cdot p$ eigenproblems of heterostructures. The new version of FTM collects merits of both BF operator ordering and the inborn cut-off method in FTM, and is robust in tackling the problem of spurious solutions encountered by $k \cdot p$ calculation. It is verified that the situation of spurious solutions met by FTM is similar to that by FEM, except that FTM has easy and simple control via N_{tr} , and thus we believe that the origin of spurious solutions is in the $k \cdot p$ theory itself rather than numerical schemes. BF operator ordering is capable enough of reject-

ing spurious solutions in the six-band calculation independently without considering the control of N_{tr} , but not in the eight-band computation, where spurious solutions exist in CB. Such incapability may be caused by the coupling of CB and VB. Proper Fourier truncation confines the Fourier series of envelope functions within the first Brillouin zone, and in practice a proper order of Fourier truncation can be chosen for sufficiently good computation accuracy and competence to prevent spurious solutions.

Taking the advantage of the intrinsic cut-off characteristic, the Fourier transform technique can screen away spurious solutions without changing any material parameters and the consideration of specific boundary conditions. The determination of the cut-off point is much more convenient than that introduced by Lassen *et al.*,¹⁴ therefore, the inborn cut-off method in FTM and BF operator ordering complements each other nicely to ease the spurious solution situation met in the $k \cdot p$ calculation. Our results suggest that BF operator ordering is indeed needed to resist spurious solutions in the six-band $k \cdot p$ computation, whereas the inborn cut-off in FTM is simple and effective to reject spurious solutions in the eight-band $k \cdot p$ computation.

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APPENDIX: DERIVATION OF FTM WITH BF OPERATOR ORDERING

We derive here the formulation of Hamiltonian matrix with BF operator ordering in the Fourier domain, with the QW as the illustration example. For the QWs, differential operations are usually used to treat with k_z in the position-dependent bulk Hamiltonians, then the Eq. (10) can be rewritten as

$$\mathbf{H}(\mathbf{r}; \mathbf{k}_{\parallel}, \hat{k}_z) \mathbf{F}(\mathbf{r}) = E(\mathbf{k}) \mathbf{F}(\mathbf{r}). \quad (\text{A1})$$

Therefore, the Hamiltonian matrix $\mathbf{H}(\mathbf{r}; \mathbf{k}_{\parallel}, \hat{k}_z)$ can be expanded with Fourier series,

$$\begin{aligned} H &= H^{(zz)}(z) \hat{k}_z^2 + H_L^{(z)}(z) \hat{k}_z + \hat{k}_z H_R^{(z)}(z) + H^{(0)}(z) \\ &= \sum_q \tilde{H}_q^{(zz)} e^{iq \cdot k_z \cdot z} \hat{k}_z^2 + \sum_q \tilde{H}_{q,L}^{(z)} e^{iq \cdot k_z \cdot z} \hat{k}_z + \sum_q \hat{k}_z \tilde{H}_{q,R}^{(z)} e^{iq \cdot k_z \cdot z} \\ &\quad + \sum_q \tilde{H}_q^{(0)} e^{iq \cdot k_z \cdot z}, \end{aligned} \quad (\text{A2})$$

where q represents the Fourier frequency the quantized z direction.

Denoting $\langle f_2 | f_1 \rangle = (1/L) \int_L f_2^* f_1 dz$, it can be derived from Eq. (A1) that,

$$\sum_{v=1}^V \sum_{n_z} c_{v,n_z} \sum_q \langle AA | \mathbf{H} | BB \rangle = \left\langle AA \left| E \sum_{v=1}^V \sum_{n_z} c_{v,n_z} \cdot BB \right. \right\rangle, \quad (\text{A3})$$

where

$$\begin{aligned} AA &= e^{ik_x x + ik_y y} e^{im_z \kappa_z z} \\ BB &= e^{ik_x x + ik_y y} e^{in_z \kappa_z z}, \end{aligned} \quad (\text{A4})$$

and $u, v = 1, 2, \dots, V$. With BF operator ordering and $\hat{k}_i \rightarrow -i\partial_i$ and $\hat{k}_j \rightarrow -i\partial_j$, we have,

$$\sum_q \langle AA | \hat{k}_z H^{(zz)}(z) \hat{k}_z | BB \rangle = \tilde{H}_{uv,q=m-n}^{(zz)} (k_z + m_z \kappa_z) (k_z + n_z \kappa_z), \quad (\text{A5})$$

$$\sum_q \langle AA | H_L^{(z)}(z) \hat{k}_z | BB \rangle = \tilde{H}_{uv,q=m-n,L}^{(z)} (k_z + n_z \kappa_z), \quad (\text{A6})$$

$$\sum_q \langle AA | \hat{k}_z H_R^{(z)}(z) | BB \rangle = \tilde{H}_{uv,q=m-n,R}^{(z)} (k_z + m_z \kappa_z), \quad (\text{A7})$$

$$\sum_q \langle AA | H^{(0)}(z) | BB \rangle = \tilde{H}_{uv,q=m-n}^{(0)}. \quad (\text{A8})$$

Therefore, we form the expectation equation, $\mathbf{M}_{um,vn} \mathbf{c}_{vn} = E \mathbf{c}_{vn}$, where the matrix element for QW is

$$\begin{aligned} \mathbf{M}_{um,vn} &= \tilde{H}_{uv,q=m-n}^{(zz)} (k_z + m_z \kappa_z) (k_z + n_z \kappa_z) \\ &\quad + \tilde{H}_{uv,q=m-n,L}^{(z)} (k_z + n_z \kappa_z) \\ &\quad + \tilde{H}_{uv,q=m-n,R}^{(z)} (k_z + m_z \kappa_z) \\ &\quad + \tilde{H}_{uv,q=m-n}^{(0)}. \end{aligned} \quad (\text{A9})$$

In the similar way, the momentum matrix for heterostructures can be expressed as

$$\begin{aligned} \mathbf{M}_{um,vn} &= \sum_{\alpha,\beta} \tilde{H}_{uv,q_i=m_i-n_i}^{(\alpha\beta)} (k_\alpha + m_\alpha \kappa_\alpha) (k_\beta + n_\beta \kappa_\beta) \\ &\quad + \sum_\alpha \tilde{H}_{uv,q_i=m_i-n_i,L}^{(\alpha)} (k_\alpha + n_\alpha \kappa_\alpha) \\ &\quad + \sum_\alpha \tilde{H}_{uv,q_i=m_i-n_i,R}^{(\alpha)} (k_\alpha + m_\alpha \kappa_\alpha) \\ &\quad + \tilde{H}_{uv,q_i=m_i-n_i}^{(0)}. \end{aligned} \quad (\text{A10})$$

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