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<th>Fourier transform-based kp method of semiconductor superlattice electronic structure</th>
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I. INTRODUCTION

In the effective mass approximation (EMA),

electron

and hole energy states in a bulk crystal are determined by solving an eigenproblem using a bulk Hamiltonian \( H_0 \). A superlattice may have abrupt interfaces, or graded composition modulation without sharp interfaces. In the former case, the eigenfunctions are found by matching wave functions in each of the constituent materials at the superlattice interfaces. In the latter, electronic states have to be calculated via numerical approaches since the explicit Hamiltonian \( H(k) \) has been developed for electronic structure calculation of superlattices. These numeric methods may also work for the superlattices with abrupt interfaces, whereas with specific consideration of the interface matching condition, no significant difference in results has ever been reported.

In a periodic superlattice, the envelope function can be approximated by a Fourier series. However, a similar treatment is applicable to the spatially varying Hamiltonian \( H(r) \) as well. The Hamiltonian in a Fourier domain for the eigenproblem can be formulated in a simple and neat form using the Fourier series of the spatial domain Hamiltonian. For arbitrary periodic structures, Fourier series expansion is implemented numerically by fast Fourier transform (FFT). Therefore, no cumbersome calculation on integral or differential is involved. Since the eigenfunction and its derivative possess a continuity property natively, it is manifest that this method is applicable to the superlattices with abrupt interfaces. In this article, we present the multiband \( k \cdot p \) Fourier transform method (FTM). The formulas of the FTM are derived and the solutions in several examples are given for illustration. Comparison is made between the FTM and FDM as well. Finally, the formulation is further extended to the case of quantum dot (QD) superlattices. To achieve high accuracy, the FDM results in a very large Hamiltonian matrix, which is challenging to solve practically. For three-dimensional heterostructures, complicated formulations in both the FDM and FEM make programming tasks challenging. In contrast, it is seen that the FTM is advantageous to overcome issues in these aspects.

II. FORMULATION FOR QW SUPERLATTICE

For the electron wave function written as

\[
\psi(r) = \sum_{v} F_v(r)u_{0v}(r),
\]

where \( u_{0v} \) is the Bloch basis with lattice periodicity, \( V \) is the number of bands involved in the model, and \( F_v(r) \) is the envelope function, it has been shown that the envelope function equation for heterostructures can be obtained from position-dependent bulk Hamiltonians \( H(r;k) \) with several operations, such as replacing \( k_z \)-related terms into differential operators,

\[
H(r;k_z)F(r) = EF(r).
\]

If the envelope function is expanded in plane waves, the eigenproblem can be solved in the form of integral-differential equations by utilizing the orthogonality of plane waves, which is to be discussed below.

For a quantum well (QW) superlattice, the envelope function is expanded in plane waves in \( z \),

\[
F(r) = e^{ik_zz}e^{i(k_x x+k_y y)}(1/L)\sum_{n} c_n e^{in\bar{L}z},
\]

where \( L \) is the period, \( c_\alpha = [c_1,c_2,\cdots,c_{\bar{L}}]^T \), \( \kappa = 2\pi/L \), and \(-\kappa < k_z \leq \kappa \). Only wave-vectors in the first Brillouin zone need be included in the expansion for uniqueness. If there are \( N \) superlattice periods, the Born–Von Karman cyclic boundary conditions give

\[
k_z = \frac{2\pi j}{NL}, \quad 0 \leq j < N.
\]

The plane waves keep their forms of complex exponential functions after operation by the operators contained in the Hamiltonian, whereas complex exponential functions possess orthogonality. Therefore, potentially the computation
will be simplified if the \( z \)-dependent Hamiltonian matrix is expanded in Fourier series as well,

\[
H = H^{(2)}(z) \hat{k}_z^2 + H^{(1)}(z) \hat{k}_z + H^{(0)}(z) \\
= \left[ \sum_q H^{(2)}(q) e^{iq\hat{k}_z} \right] \hat{k}_z^2 + \left[ \sum_q H^{(1)}(q) e^{iq\hat{k}_z} \right] \hat{k}_z + \sum_q H^{(0)}(q) e^{iq\hat{k}_z} \\
\times (q) e^{iq\hat{k}_z}.
\]

(4)

Denoting \( \langle f_2 | f_1 \rangle = (1/L) \int f_2^* f_1 dz \), it can be derived from Eq. (2) that

\[
\langle e^{i(k_m + n)z} | \sum_{n=1}^{V} \left[ \sum_{q} \left[ e^{iq\hat{k}_z} H^{(2)}(q) e^{iq\hat{k}_z} \right] e^{i(k_m + n)z} \right] \\
+ \langle e^{i(k_m + n)z} | \sum_{n=1}^{V} \left[ \sum_{q} \left[ e^{iq\hat{k}_z} H^{(1)}(q) e^{iq\hat{k}_z} \right] e^{i(k_m + n)z} \right] \\
+ \langle e^{i(k_m + n)z} | \sum_{n=1}^{V} \left[ \sum_{q} \left[ e^{iq\hat{k}_z} H^{(0)}(q) e^{iq\hat{k}_z} \right] e^{i(k_m + n)z} \right] \rangle \\n= \langle e^{i(k_m + n)z} | \sum_{n=1}^{V} \left[ \sum_{q} \left[ c_{vn} e^{i(k_m + n)z} \right] \right].
\]

(5)

\[
\sum_{n=1}^{V} \sum_{q} c_{vn} \left[ \sum_{q} \left[ e^{iq\hat{k}_z} H^{(2)}(q) e^{iq\hat{k}_z} \right] e^{i(k_m + n)z} \right] \\
+ \langle e^{i(k_m + n)z} | \sum_{n=1}^{V} \left[ \sum_{q} \left[ e^{iq\hat{k}_z} H^{(1)}(q) e^{iq\hat{k}_z} \right] e^{i(k_m + n)z} \right] \\
+ \langle e^{i(k_m + n)z} | \sum_{n=1}^{V} \left[ \sum_{q} \left[ e^{iq\hat{k}_z} H^{(0)}(q) e^{iq\hat{k}_z} \right] e^{i(k_m + n)z} \right] \rangle \\
= E \sum_{n=1}^{V} \sum_{q} c_{vn},
\]

(6)

where \( u=1,2,\ldots,V \). We adopted an eight-band \( k \cdot p \) Hamiltonian in this work. With the Hermitian operation, \( \hat{k}_z \rightarrow [Q \hat{k}_z + \hat{k}_z(Q)]/2 \) and \( \hat{k}_z \rightarrow [Q \hat{k}_i + \hat{k}_i(Q)]/2 \), where \( \hat{k}_z \rightarrow i\hat{k}_z \) and \( \hat{k}_z \rightarrow -i\hat{k}_z \), we have

\[
\sum_{q} \left( e^{i(k_m + n)z} \right) H^{(0)}(q) e^{iq\hat{k}_z} = H^{(0)}(q) = H^{(0)}(q = m - n),
\]

(7)

\[
\sum_{q} \left( e^{i(k_m + n)z} \right) H^{(2)}(q) e^{iq\hat{k}_z} = \left( \frac{km + kn}{2} + k_z \right) H^{(2)}(q = m - n),
\]

(8)

\[
\sum_{q} \left( e^{i(k_m + n)z} \right) H^{(1)}(q) e^{iq\hat{k}_z} = \left( km + k_n \right) H^{(1)}(q = m - n).
\]

(9)

Therefore, the equation for the eigenproblem can be written as

\[
[M_{ST}][c] = [E][c],
\]

(10)

where the matrix elements of Fourier domain Hamiltonian \( M \) have the following expression:

\[
M_{ST} = \left( \frac{km + kn}{2} + k_z \right) H^{(2)}(q = m - n) v + \sum_{q} \left( e^{i(k_m + n)z} \right) H^{(1)}(q = m - n).
\]

III. ELECTRONIC STRUCTURE CALCULATION

To illustrate the FTM calculation, three structures are employed: a 35 Å InGaAs/300 Å InP abrupt QW (denoted as AQW), a 35 Å InGaAs/400 Å InP QW being intermixed with 5 Å diffusion length on both sublattices (denoted as IQW), and a short-period superlattice 35 Å InGaAs/400 Å InP (denoted as SSL). The results obtained by the FTM are shown in Fig. 1 and the FDM results are presented as references in Figs. 1(a) and 1(b) as well. The calculation adopts the band parameters from Table I in Ref. 12. The IQW structures are sliced with 512 mesh points for both FTM and FDM calculations. In the FTM calculation, a FFT is done with the mesh and the truncation frequency is \( N=20 \) for forming the Fourier domain Hamiltonian. It is seen that the calculation results using these two methods agree with each other nicely.

In the FDM calculation, we did not have specific consideration of the interface matching condition for the reason stated as above. The FDM can incorporate the interface
matching condition only for heterostructures with abrupt interfaces, e.g., AQW, but not for heterostructures with graded composition, e.g., IQW. For the circumstance of FTM, the interface matching condition cannot be intentionally incorporated because abrupt interfaces no longer exist in Fourier series approximation as shown in Fig. 2.

In some works, e.g., Ref. 13, the eigenvalue equation only adopts the bulk Hamiltonian of the QW layer’s constitutional material and treats band offsets with a perturbation term in a form like

\[ H(z) = H(0) + U(z), \]

where \( U(z) \) is diagonal in the basis and describes only the valence and conduction band offsets. The influence of such an approximation to accuracy can be evaluated in FTM calculation. The \( E-k \) plots in Fig. 1 show that the deviation due to this approximation goes large for large \( k \). A basic understanding is that such an approximation neglects the spatial variation of the band parameters, i.e., \( \gamma_1, \gamma_2, \gamma_3, \gamma_4, \) and \( \Delta \), and brings an appreciable error when band mixing goes large, i.e., large \( k \). However, for a short-period superlattice, since the envelope function is not small over the barrier region, neglecting the spatial variation of band parameters will bring an appreciable deviation even at \( k=0 \). The \( E-k \) plot of SSL in Fig. 1(c) shows \( \sim 4 \) meV deviation in \( E_1 \) at \( k=0 \).

Under EMA, the FTM is derived without extra approximations or assumptions. However, for numerical calculation, a structure has to be meshed for performing a FFT if analytical expressions of the Fourier series are neither available nor adopted. Furthermore, the Fourier series need be truncated to make finite the Fourier domain Hamiltonian \( \mathbf{M} \). Both meshing and truncation are factors causing numerical errors. Unlike the FDM, increasing mesh density does not cause a significant rise of the computing volume in the FTM, owing to the specific feature of the FFT algorithm. In comparison to the discretization-caused numerical error, which can be easily reduced, it takes more cost to reduce the truncation-caused numerical error. In Fig. 2, we can see that the truncated Fourier series deviates from the original band edge profile, and the influences are different between heterostructures with abrupt interfaces and those with graded compositions. As shown in Fig. 3, to reach an accuracy of \( \sim 1 \) meV, the truncation frequency \( N \) should be no less than 20, 14, and 5 for AQW, IQW, and SSL, respectively. The reason why the greatest \( N \) is needed for AQW but the smallest \( N \) for SSL to reach the same accuracy can be explained using the Fourier spectra shown in Fig. 4. AQW has a widespread spectrum compared to the others, whereas the spectrum of SSL has very large magnitudes only at the first several frequencies. The spectrum of IQW has the narrowest span, and thus the best accuracy can be achieved when \( N \) further increases, as seen in Fig. 3(b). A 512-point mesh is used to perform a FFT for the plots in Fig. 3.

Discretization-caused numerical error is investigated in
eigenvalues versus \( N_p \) solved by the FDM and the eigenvalues versus \( 2N+1 \) solved by the FTM for AQW and IQW, respectively. Comparison is done under the same dimension of the Hamiltonian matrix. \( N_p \) influences the accuracy to a different extent for different heterostructures. The FDM curve for AQW in Fig. 6 shows zigzag patterns swinging in ranges of 3–7 meV even for \( N_p > 500 \). This is due to edge jitter of the mesh near abrupt interfaces along with increasing \( N_p \), which is equivalent to the fluctuation of the well width. This phenomenon is not observable in a graded QW like IQW once \( N_p \) is sufficiently large.

However, to further improve the accuracy in the FDM, more mesh points have to be pursued. In reality, the challenge is that the matrix may become too big to solve, because the matrix dimension is determined by the number of mesh points, i.e., \( VN_p \times VN_p \). In contrast, the dimension of the Hamiltonian matrix used in the FTM [Eqs. (10) and (11)] is subjective to \( N \), i.e., \( V(2N+1) \times V(2N+1) \). From the above results, it is seen that to reach an accuracy of \( \sim 1 \) meV, \( N = 20 \) is sufficient for all three cases. When more mesh points are needed to reduce the discretization-caused error, the FTM only brings more computation volume to the FFT, for which the increase in computing time is trivial. Apparently the FTM is much more efficient than the FDM, especially in dealing with abrupt QWs, as has also been manifested in the practical computation.

V. FORMULATION FOR QD SUPERLATTICE

The FTM presents a simple and neat formulation for the QW superlattice in Eq. (11). It brings the same advantage to the QD superlattice as well. The envelope function for a QD superlattice as well. The envelope function for a QD superlattice in Eq. (14) may be even less than 128 for IQW. AQW and IQW, respectively. Comparison is done under the same dimension of the Hamiltonian matrix used in the FTM [Eqs. (10) and (11)] is subjective to \( N \), i.e., \( V(2N+1) \times V(2N+1) \). From the above results, it is seen that to reach an accuracy of \( \sim 1 \) meV, \( N = 20 \) is sufficient for all three cases. When more mesh points are needed to reduce the discretization-caused error, the FTM only brings more computation volume to the FFT, for which the increase in computing time is trivial. Apparently the FTM is much more efficient than the FDM, especially in dealing with abrupt QWs, as has also been manifested in the practical computation.

V. FORMULATION FOR QD SUPERLATTICE

The FTM presents a simple and neat formulation for the QW superlattice in Eq. (11). It brings the same advantage to the QD superlattice as well. The envelope function for a QD superlattice is expressed as

\[
F(r) = \frac{1}{\sqrt{L_x L_y L_z}} e^{i \vec{k} \cdot \vec{r}} \sum_{n_x=-N_x}^{N_x} \sum_{n_y=-N_y}^{N_y} \sum_{n_z=-N_z}^{N_z} c_{n_x n_y n_z} e^{i (n_x k_x + n_y k_y + n_z k_z)}.
\]

where \( L_x, L_y, \) and \( L_z \) are the structural periods; \( c_{n_x n_y n_z} \) is the amplitude of the eigenfunction, \( k_x = 2 \pi / L_x \), \( k_y = 2 \pi / L_y \), and \( -k_x < k_x < k_x \). \( r = x, y, \) and \( z \).

The spatial domain Hamiltonian matrix is expressed in the Fourier domain using Fourier transform

\[
H = \sum_{a, \beta, \mu, \nu, \lambda} H^{a \beta}(x, y, z) \hat{k}^a \hat{k}^\beta + \sum_{a, \mu, \nu, \lambda} H^a(x, y, z) \hat{k}_a + H^0(x, y, z)
\]

\[
= \sum_{a, \beta, \mu, \nu, \lambda} H^{a \beta}(x, y, z) \hat{k}^a \hat{k}^\beta + \sum_{a, \mu, \nu, \lambda} H^a(x, y, z) \hat{k}_a + H^0(x, y, z)
\]

Denoting \( \langle f_1 | f_2 \rangle = \int V \int f_1^* f_2 d\Omega \), the eigenvalue equation \( HF = EF \) gives

\[
\int f_1^* f_2 d\Omega = \frac{1}{V} \sum_{a, \beta} H^{a \beta}(x, y, z) \langle \hat{k}^a \hat{k}^\beta \rangle + \sum_{a} H^a(x, y, z) \langle \hat{k}_a \rangle + H^0(x, y, z) \langle f_2 \rangle = \lambda \langle f_2 \rangle.
\]
With Hermitian operation, the matrix element for the eigenvalue equation [Eq. (10)] can be obtained,

\[
M = \frac{1}{2} \sum_{\alpha, \beta} [2k_\alpha k_\beta + k_\alpha (m_\beta + n_\beta) \kappa_\beta + k_\beta (m_\alpha + n_\alpha) \kappa_\alpha + (m_\alpha n_\beta + m_\beta n_\alpha) \kappa_\alpha \kappa_\beta] H_{\alpha \beta}^{\alpha, \beta} (q_x, q_y, q_z) + \sum_{\alpha} [2k_\alpha] + (m_\alpha + n_\alpha) \kappa_\alpha H_{\alpha \alpha}^{\alpha, \alpha} (q_x, q_y, q_z) + H_{\alpha \alpha}^{\alpha, \alpha} (q_x, q_y, q_z),
\]

(16)

where \(q_x = m_x - n_x, q_y = m_y - n_y, \) and \(q_z = m_z - n_z.\)

VI. CONCLUSION

We have presented the FTM for solving multiband \(k \cdot p\) eigenproblems of heterostructures. The Fourier domain Hamiltonian expressed in a simple and neat form is derived from the position-dependent Hamiltonian in a spatial domain. The dimension of the Hamiltonian used in the FTM is determined by the truncation frequency \(N\) only. In case analytical expressions of the Fourier series are not given, a dense mesh can be adopted to reduce the discretization-caused numerical error with trivial increase of computing time. Therefore, the FTM is numerically efficient in solving multiband \(k \cdot p\) eigenproblems. This advantage is more prominent for a heterostructure with abrupt interfaces. Approximation by adopting the QW layer’s bulk Hamiltonian with a perturbation term for band offsets may lead to large deviation for large \(k\) in long-period superlattices and even at zero \(k\) in short-period superlattices. Furthermore, the FTM presents a simple and neat formulation for the QD eigenproblems as well.

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