Position-dependent effective masses in semiconductor theory. II

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We consider a compound semiconductor possessing a slowly varying position-dependent chemical composition. We derive an effective-mass equation governing the dynamics of electron (or hole) motion using the Kohn-Luttinger representation and canonical transformations. We show that, as long as the variation in chemical composition may be treated as a perturbation, the effective masses become constant, position-independent quantities. The effective-mass equation derived here is identical to the effective-mass equation derived previously by von Roos, using a Wannier representation.

I. INTRODUCTION

Effective-mass equations applicable to graded, mixed semiconductors have been derived by several authors.[1] In all cases the variation of the chemical composition (the grading) was considered to be slow enough so that changes of composition become appreciable only over distances large compared to the lattice constant. Gora and Williams[1] (GW) as well as van Vliet and Marshak[1] (VVM) start with the Schrödinger equation of the compound semiconductor in the Wannier representation as did von Roos (VR).[1] During the course of the derivation a certain matrix element appears which was manipulated in a different way by these authors. Here is not the place to go into the details of the algebra. The reader is urged to consult the original literature.[1] The effective masses derived by GW as well as VVM exhibited explicitly a position dependence, whereas the effective masses derived by VR did not.[1] It was later shown that the GW or VVM effective-mass Hamiltonians are not unique.[2] This fact was later disputed.[3] But as was pointed out by Morrow[3] the nonuniqueness of the GW and VVM Hamiltonians still persist when the wavelengths of the envelope functions are not small compared with the distance over which the chemical composition changes appreciably. But this is precisely the case for wave functions of excited shallow impurity states which extend over hundreds of lattice sites. The derivation by VR is, however, unique.[1] We now come to the work of Leibler.[1] Rather than using a Wannier representation, he proceeded to derive an effective-mass equation for graded semiconductor material with the aid of the Kohn-Luttinger (KL) method.[4] Leibler's calculations resulted in an effective-mass equation for the envelope function which is quite similar to the corresponding equations of GW and VVM, but not identical with either. Again, the effective masses became position dependent. The KL method[4] leads to a unique result and should therefore lead to the same result as VR,[1] in particular to position-independent (constant) effective masses.[5] We have therefore investigated this problem again, using the KL technique and found a number of mathematical and physical errors in Leibler's work. Eliminating these errors, we can show that the KL method[4] leads to the same result as the derivation by VR.[1] This we shall do in the next section.

II. THEORY

We start with the Hamiltonian of a binary alloy in the one-electron approximation:

$$H=-\frac{\hbar^2}{2m}\nabla^2+f(\mathbf{r})V_A(\mathbf{r})+[1-f(\mathbf{r})]V_B(\mathbf{r})+U(\mathbf{r}) , \quad (1)$$

where $f(\mathbf{r})$ is the position-dependent concentration of A atoms in a regular lattice consisting of A and B atoms, and U is a slowly varying potential. To facilitate comparison with Leibler's work,[1] we use largely his notation. The Hamiltonian (1) has been used by Leibler[1] and independently by von Roos[1] and the reader is referred to these references for details. If $f=f_0=$ const and $U=0$, the Hamiltonian (1) would be periodic in the underlying Bravais lattice. With a suitably chosen f_0, the Hamiltonian (1) may be rewritten as

$$\begin{aligned} H&=-\frac{\hbar^2}{2m}\nabla^2+f_0V_A+(1-f_0)V_B \\ &\quad+[f(\mathbf{r})-f_0](V_A-V_B)+U \\ &=H_0+L(\mathbf{r})S(\mathbf{r})+U(\mathbf{r}) \end{aligned} \quad (2)$$

with $L=f-f_0$ and $S=V_A-V_B$. For a sufficiently slowly varying composition, $f-f_0$ may be considered small and the term LS of Eq. (2) may be treated as a perturbation. By writing the Hamiltonian in the form given by Eq. (2), we have managed to split the Hamiltonian (1) into a large, periodic part H_0 and a small nonperiodic part $LS+U$. The task we are confronted with now, consists in solving Schrödinger's equation

$$H\psi=(H_0+LS+U)\psi=E\psi , \quad (3)$$

where E is the total energy of the system. We now proceed with Leibler[1] to introduce the set of Kohn-Luttinger functions[4]

$$\xi_{n\mathbf{k}}=e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{n\mathbf{k}_0}=|n,\mathbf{k}\rangle\ , \tag{4}$$

where the Bloch functions $\psi_{n\mathbf{k}_0}$ satisfy

$$H_0\psi_{n\mathbf{k}_0}=E_n(\mathbf{k}_0)\psi_{n\mathbf{k}_0}\ . \tag{5}$$

We assume further that there exists a simple minimum of the band energy E_n at $\mathbf{k}=\mathbf{k}_0$.

Expanding ψ of Eq. (3) into the complete orthonormal set of Kohn-Luttinger functions, with

$$\psi=\sum_{n,\mathbf{k}}A_n(\mathbf{k})\,|n,\mathbf{k}\rangle \tag{6}$$

we obtain from Eq. (3) the set of equations

$$\sum_{n'\mathbf{k}'}\langle n,\mathbf{k}\,|\,H\,|\,n',\mathbf{k}'\rangle A_{n'}(\mathbf{k}')=EA_n(\mathbf{k})\ . \tag{7}$$

The Hamiltonian H consists of three parts according to Eq. (3). The matrix elements of the unperturbed Hamiltonian H_0 are given by

$$\begin{aligned}\langle n,\mathbf{k}\,|\,H_0\,|\,n',\mathbf{k}'\rangle&=\left[E_n(\mathbf{k}_0)+\frac{\hbar^2k^2}{2m}\right]\delta_{nn'}\delta_{\mathbf{k}|\mathbf{k}'}\\&\quad+\lambda_1\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}_{nn'}\delta_{\mathbf{k}|\mathbf{k}'}\\&=H^0_{n\mathbf{k}|n'\mathbf{k}'}+\lambda_1H^1_{n\mathbf{k}|n'\mathbf{k}'}\\&=H^0+\lambda_1H^1\ .\end{aligned} \tag{8}$$

Here $\mathbf{p}_{nn'}$ is defined by

$$\mathbf{p}_{nn'}=\int\psi^*_{n\mathbf{k}_0}\frac{\hbar}{i}\nabla\psi_{n'\mathbf{k}_0}d^3r \tag{9}$$

with the important property

$$\mathbf{p}_{nn}=0\ , \tag{10}$$

since we have assumed a minimum of E_n at $\mathbf{k}=\mathbf{k}_0$.[4]

The constant λ_1 has been introduced for convenience. Since we will perform successive canonical transformations later on, it is indeed convenient to keep track of terms of order λ_1, λ_1^2, etc. After all calculations are done, λ_1 may be set equal to 1. The matrix elements of the remaining terms of the Hamiltonian (3) are given by

$$\langle n,\mathbf{k}\,|\,LS\,|\,n',\mathbf{k}'\rangle=v_{nn'}\mathscr{L}(\mathbf{k}-\mathbf{k}')\ , \tag{11}$$

where

$$v_{nn'}=\int d^3r\,S\psi^*_{n\mathbf{k}_0}\psi_{n'\mathbf{k}_0} \tag{12}$$

and the Fourier transform of L is denoted by $\mathscr{L}$, viz.,

$$\mathscr{L}(\mathbf{k})=\frac{1}{V}\int e^{-i\mathbf{k}\cdot\mathbf{r}}L(\mathbf{r})d^3r\ , \tag{13}$$

where V is the quantization volume. Equation (11) is valid if L is slowly varying (see Leibler for details[1]). Finally,

$$\langle n,\mathbf{k}\,|\,U\,|\,n',\mathbf{k}'\rangle=\mathscr{U}(\mathbf{k}-\mathbf{k}')\delta_{nn'} \tag{14}$$

provided that U is also slowly varying.[4] Again, $\mathscr{U}$ is the Fourier transform of U, viz.,

$$\mathscr{U}(\mathbf{k})=\frac{1}{V}\int e^{-i\mathbf{k}\cdot\mathbf{r}}U(\mathbf{r})d^3r\ . \tag{15}$$

It is now convenient to split the matrix element (11) into diagonal and off-diagonal elements in the band indices

$$\mathscr{L}(\mathbf{k}-\mathbf{k}')v_{nn'}=\mathscr{L}(\mathbf{k}-\mathbf{k}')[\lambda_3v_{nn}\delta_{nn'}+\lambda_2v_{nn'}(1-\delta_{nn'})]\ . \tag{16}$$

The constants λ_2 and λ_3 have been introduced for the same reason as the constant λ_1 above. We define

$$H^2=H^2_{n\mathbf{k}|n'\mathbf{k}'}=\mathscr{L}(\mathbf{k}-\mathbf{k}')v_{nn'}(1-\delta_{nn'})\ . \tag{17}$$

Introducing a compact notation, we obtain as a starting point the following expression for Eq. (7):

$$HA=(H^0+\lambda_1H^1+\lambda_2H^2+\lambda_3V^1+\mathscr{U})A=EA\ . \tag{18}$$

Equation (18) constitutes a matrix equation. We have omitted all matrix indices, so, for instance, $\mathscr{U}A$ stands for

$$\begin{aligned}\mathscr{U}A&=\sum_{n'\mathbf{k}'}\mathscr{U}_{n\mathbf{k}|n'\mathbf{k}'}A_{n'}(\mathbf{k}')\\&=\sum_{\mathbf{k}'}\mathscr{U}(\mathbf{k}-\mathbf{k}')A_n(\mathbf{k}')\end{aligned} \tag{19}$$

according to Eq. (14).

We note, that the matrices H^0, V^1, and $\mathscr{U}$ are diagonal in the band index, whereas H^1 and H^2 possess off-diagonal elements *only*. So far, the problem at hand has only been *defined* by Eq. (18) and nothing new has yet emerged. In fact, Eq. (18) constitutes the starting point of Leibler's further analyses.[1] For the clarity of exposition and for the comfort of the reader, we felt it worthwhile to explain once more the steps which led to Eq. (18) and to define concisely all quantities involved.

In order to eliminate the interband matrix elements H^1 and H^2 from the Hamiltonian H of Eq. (18) we proceed, with KL (Ref. 4) and Leibler (Ref. 1), to introduce a canonical transformation, which removes the interband terms H^1 and H^2 to first order. With

$$B=e^{-T}A\ , \tag{20a}$$

it follows that

$$e^{-T}He^{T}B=H_{\text{eff}}B=EB\ , \tag{20b}$$

from Eq. (18). We expand the effective Hamiltonian H_{eff} in commutators

$$H_{\text{eff}}=H+[H,T]+\tfrac{1}{2}[[H,T],T]+\cdots\ , \tag{21}$$

and put with Leibler (Ref. 1)

$$T=T^1+T^2\ . \tag{22}$$

Stipulating that

$$[H^0,T^1]=-\lambda_1H^1\ , \tag{23a}$$

$$[H^0,T^2]=-\lambda_2H^2\ , \tag{23b}$$

we have eliminated the first-order interband matrix elements as promised. The solutions to Eqs. (23) are given by

$$T^1=-\lambda_1\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}_{nn'}E^{-1}_{nn'}\delta_{\mathbf{k}|\mathbf{k}'}\ , \tag{24a}$$

and

$$T^2=-\lambda_2 v_{nn'}\mathscr{L}(\mathbf{k}-\mathbf{k}')\epsilon^{-1}_{n\mathbf{k}|n'\mathbf{k}'}\ . \tag{24b}$$

Here, $T^1_{nn}=T^2_{nn}=0$ and the energy denominators are defined by

$$\epsilon^{-1}_{n\mathbf{k}|n'\mathbf{k}'}=\left[E_n(\mathbf{k}_0)+\frac{\hbar k^2}{2m}-E_{n'}(\mathbf{k}_0)-\frac{\hbar^2(k')^2}{2m}\right]^{-1} \tag{25a}$$

and

$$E^{-1}_{nn'}=\epsilon^{-1}_{n\mathbf{k}|n'\mathbf{k}}\ . \tag{25b}$$

For wide-band-gap semiconductors and for sufficiently slowly varying chemical composition, both T^1 and T^2 may be considered as small compared to 1 [Eqs. (30) and (32) of Leibler[1]]. In this case, the only terms which should be retained in the expansion, Eq. (21), other than the zero-order terms, are those proportional to λ_1^2, $\lambda_1\lambda_2$, and $\lambda_1\lambda_3$. Terms of the order of λ_2^2 and $\lambda_1^2\lambda_2$ should be neglected. The former, those of order λ_2^2, being proportional to $\mathscr{L}^2$ have consistently been neglected by Leibler, but the latter, those of order $\lambda_1^2\lambda_2$, have been retained by Leibler. This procedure is inconsistent, since by the same token, terms of order λ_1^3 should also be retained, terms, which, however, have been discarded by Leibler (Ref. 1) on the same grounds as was argued by Luttinger and Kohn.[4]

Retaining then only terms up to order λ_1^2, $\lambda_1\lambda_2$, and $\lambda_1\lambda_3$, the effective Hamiltonian matrix (21) becomes, using T^1 and T^2 defined in Eqs. (24),

$$\begin{aligned}H_{\text{eff}}=&H^0+\lambda_3V^1+\mathscr{U}+\lambda_1\frac{\hbar}{m}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{p}_{nn'}\mathscr{U}(\mathbf{k}-\mathbf{k}')\epsilon^{-1}_{n\mathbf{k}|n'\mathbf{k}'}+\lambda_1^2\frac{\hbar^2}{2m^2}\sum_{n''}\mathbf{k}\cdot\mathbf{p}_{nn''}\mathbf{k}\cdot\mathbf{p}_{n''n'}(E^{-1}_{nn''}+E^{-1}_{n'n''})\delta_{\mathbf{k}|\mathbf{k}'}\\&+\lambda_1\lambda_3\frac{\hbar}{m}(v_{n'n'}\mathbf{k}-v_{nn}\mathbf{k}')\cdot\mathbf{p}_{nn'}\mathscr{L}(\mathbf{k}-\mathbf{k}')E^{-1}_{nn'}\\&+\lambda_1\lambda_2\frac{\hbar}{2m}\sum_{n''}[\mathbf{k}\cdot\mathbf{p}_{nn''}v_{n''n'}(1-\delta_{n''n'})(E^{-1}_{nn''}+\epsilon^{-1}_{n'\mathbf{k}'|n''\mathbf{k}})+\mathbf{k}'\cdot\mathbf{p}_{n''n'}v_{nn''}(1-\delta_{nn''})(\epsilon^{-1}_{n\mathbf{k}|n''\mathbf{k}'}+E^{-1}_{n'n''}]\mathscr{L}(\mathbf{k}-\mathbf{k}')\ .\end{aligned} \tag{26}$$

It is possible to eliminate the off-diagonal matrix elements linear in $\mathscr{L}$ of Eq. (26) by means of a further transformation T^3. The complete canonical transformation now becomes

$$T=T^1+T^2+T^3\ , \tag{27}$$

where T^1 and T^2 are given by Eqs. (24) and T^3 is defined by the commutator

$$\begin{aligned}[H^0,T^3]=&-\frac{\lambda_1}{2}[H^1,T^2]-\frac{\lambda_2}{2}[H^2,T^1]-\lambda_3[V^1,T^1]\\&+\lambda_1\lambda_2\frac{\hbar}{m}\mathscr{L}(0)\sum_{n''\neq n}[v_{nn''}(1-\delta_{nn''})\mathbf{p}_{n''n}+\mathbf{p}_{nn''}v_{n''n}(1-\delta_{n''n})]\cdot\mathbf{k}E^{-1}_{nn''}\delta_{nn'}\delta_{\mathbf{k}|\mathbf{k}'}\ .\end{aligned} \tag{28}$$

We note that Eq. (28) is quite similar to Leibler's expression for the additional canonical transformation T^3 [Eq. (33) of Leibler (Ref. 1)]. In fact, if we omit the last term on the right-hand side (RHS) of Eq. (28), it becomes identical with Leibler's corresponding equation. But because all matrix elements of T^3 must be finite, in fact small, and because the diagonal matrix elements of the commutator $[H^0,T^3]$ vanish, the diagonal matrix elements of the RHS of Eq. (28) must also vanish. But the first two commutators on the RHS of Eq. (28) possess nonvanishing diagonal matrix elements. They must therefore be subtracted in order to make Eq. (28) consistent. Hence we have the last term on the RHS of Eq. (28). Performing now the full transformation (27) on the original Hamiltonian defined by Eq. (18), or equivalently performing the transformation T^3 on the effective Hamiltonian (26), removes all off-diagonal elements of order $\lambda_1\lambda_2$ and $\lambda_1\lambda_3$. It does not remove the off-diagonal elements of order λ_1^2 and those containing the potential $\mathscr{U}$. But these off-diagonal elements have been shown to be small by Luttinger and Kohn (Ref. 4) and may be omitted. The final result of the calculations is then given by the following expression:[6]

$$H_{\text{eff}}=\left[E_n(\mathbf{k}_0)+\frac{\hbar^2}{2}\sum_{\alpha,\beta}\left[\frac{1}{m_n}\right]_{\alpha\beta}k_\alpha k_\beta+\frac{\hbar}{m}\mathscr{L}(0)\mathbf{k}\cdot\mathbf{b}_n\right]\delta_{\mathbf{k}|\mathbf{k}'}+\mathscr{U}(\mathbf{k}-\mathbf{k}')+v_{nn}\mathscr{L}(\mathbf{k}-\mathbf{k}')\ . \tag{29}$$

Here, k_α signifies the α component of the vector $\mathbf{k}$ in a Cartesian coordinate system. The effective-mass tensor $(m_n^{-1})_{\alpha\beta}$ of Eq. (29), identical to the Luttinger-Kohn mass tensor (Ref. 4), is defined by

$$\left[\frac{1}{m_n}\right]_{\alpha\beta}=\frac{1}{m}\delta_{\alpha\beta}+\frac{2}{m^2}\sum_{n'\neq n}E^{-1}_{nn'}p^\alpha_{nn'}p^\beta_{n'n}\ , \tag{30}$$

where $p^\alpha_{nn'}$, defined by Eq. (9), is the α component of the momentum matrix element of band n, and $E_{nn'}$ is given by Eq. (25b). The vector $\mathbf{b}_n$ in turn is given by

$$\mathbf{b}_n = \sum_{n' \neq n} E_{nn'}^{-1} (v_{nn'} \mathbf{p}_{n'n} + \mathbf{p}_{nn'} v_{n'n}) \ . \tag{31}$$

We note that the effective mass, Eq. (30), does not depend on position and represents the effective mass associated with the Hamiltonian of Eq. (5).

Using Eqs. (20a) and (27), we find that

$$B = e^{-T} A = (1 - T_1 - T_2 - T_3) A \approx A \tag{32}$$

since T_1, T_2, and T_3 are small quantities. Defining the envelope function via

$$A_n(\mathbf{k}) = \int d^3r \, F_n(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \ , \tag{33}$$

we find with the help of Eq. (29) that F_n satisfies the following Schrödinger equation:

$$\left[-\frac{\hbar^2}{2} \sum_{\alpha,\beta} \left[\frac{1}{m_n} \right]_{\alpha\beta} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} + U(\mathbf{r}) + v_{nn} L(\mathbf{r}) + \frac{\hbar}{im} \mathscr{L}(0) \mathbf{b}_n \cdot \nabla \right] F_n = (E - E_n) F_n \ . \tag{34}$$

Finally, the transformation

$$F_n = \exp[-(i/\hbar) \mathscr{L}(0) \mathbf{c}_n \cdot \mathbf{r}] G_n(\mathbf{r}) \tag{35}$$

removes the gradient term, the last term on the left-hand side of Eq. (34), provided that the vector $\mathbf{c}_n$ satisfies the set of equations

$$\sum_\beta \left[\frac{1}{m_n} \right]_{\alpha\beta} c_{n\beta} = m^{-1} b_{n\alpha} \tag{36}$$

and that quadratic terms in $\mathscr{L}$ may be neglected. Equation (36) always has a solution, since the matrix of the inverse mass tensor is nonsingular and terms of order $\mathscr{L}^2$ have been neglected throughout. With the definition (12) and the definitions for L and S given by Eq. (2), G_n satisfies

$$\left[-\frac{\hbar^2}{2} \sum_{\alpha\beta} \left[\frac{1}{m_n} \right]_{\alpha\beta} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} + U(\mathbf{r}) + W(\mathbf{r}) \right] G_n = (E - E_n) G_n \ , \tag{37}$$

where W is given by

$$W = [f(\mathbf{r}) - f_0] \int d^3r \, \psi^*_{n\mathbf{k}_0} (V_A - V_B) \psi_{n\mathbf{k}_0} \ . \tag{38}$$

Equation (37) differs from Eq. (37) of VR, Ref. 1, only in the matrix element of $V_A - V_B$. To be more specific, the expression of VR corresponding to Eq. (38) above reads

$$W = [f(\mathbf{r}) - f_0] \int d^3r \, a_n^*(\mathbf{r}) (v_A - v_B) a_n(\mathbf{r}) \ . \tag{39}$$

The connection between V_A and v_A is given by[7] [see VR (Ref. 1), Eq. (26)]

$$V_A(\mathbf{r}) = \sum_j v_A(\mathbf{r} - \mathbf{R}_j) \ , \tag{40}$$

where the sum runs over all lattice sites $\mathbf{R}_j$. The connection between the Bloch functions $\psi_{n\mathbf{k}}$ and the Wannier functions $a_n(\mathbf{r})$ occurring in Eq. (39) is well known to be

$$\psi_{n\mathbf{k}} = N^{-1/2} \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j} a_n(\mathbf{r} - \mathbf{R}_j) \tag{41}$$

with N being the number of unit cells within the quantization volume.

Inserting expressions (40) and (41) into the matrix element of Eq. (38), and utilizing the facts that the Wannier functions are localized about their lattice sites and that the potential terms $v_A(\mathbf{r} - \mathbf{R}_j)$ and $v_B(\mathbf{r} - \mathbf{R}_j)$ also tend to be large for small arguments, it can easily be shown that the matrix elements of Eqs. (38) and (39) are identical to all intents and purposes. Thus we have shown that the same effective-mass equation is obtained, regardless of the method employed to derive it.

III. SUMMARY

On the preceding pages we have shown that the effective-mass equation for semiconductor material possessing a slowly varying chemical composition, derived via the method of Luttinger and Kohn[4] is identical with the effective-mass equation derived via the Wannier-Slater method [VR (Ref. 1)]. This is in itself not surprising, were it not for the fact that a previous attempt showed otherwise [Leibler (Ref. 1)]. However, we have exhibited in Sec. II a number of errors (retention of higher order terms inconsistently and incorrect commutator relations) in that work, which, when corrected, led to the expected equivalence of the effective-mass equations. Within the approximations involved, essentially the same as those discussed by Luttinger and Kohn as well as by Leibler, the effective-mass tensor is position independent in contrast to the findings of Gora and Williams or von Vliet and Marshak (Ref. 1). But we have shown earlier[2] that the work of these authors led to ambiguities and must therefore be rejected. It seems to us that the effective-mass equation (37) is the correct one within the framework of the underlying approximations.

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[5]To be more succinct, Eq. (37) of VR (Ref. 1) and Eq. (42) of Leibler's paper (Ref. 1) should be equivalent. The effective-mass equation given by VR, expressed in Wannier functions, should be connected to Leibler's result, expressed in Kohn-Luttinger functions, merely by a unitary transformation.

[6]We have set $\lambda_1=\lambda_2=\lambda_3=1$ in the final expression (29).

[7]A similar connection exists of course also between V_B and v_B.