Electromagnetic analogies to general-Hamiltonian effective-mass electron wave propagation in semiconductors with spatially varying effective mass and potential energy

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(Received 1 October 1991; revised manuscript received 10 December 1991)

It is shown that exact, quantitative electromagnetic analogies exist for *all* forms of the general Hamiltonian [R. A. Morrow and K. R. Brownstein, Phys. Rev. B **30**, 678 (1984)], which applies to single-band effective-mass electron wave propagation in semiconductors. It is further shown that these analogies are valid for propagation in the bulk, propagation past abrupt interfaces between materials, and propagation within one- and two-dimensionally inhomogeneous materials. These results indicate that the correct form of the single-band effective-mass Hamiltonian can be determined through appropriate wave-function-amplitude-sensitive experiments. Wave-function-phase-sensitive experiments (such as the measurement of electron wave refraction directions) are not adequate to specify completely the Hamiltonian. The present analogies suggest many wave-function-amplitude-sensitive experiments that can be used to determine the correct form of the Hamiltonian. The results of the present analysis are broadly applicable to general effective-mass propagation, unlike other recent work that has treated specific cases.

Recent advances in nanostructure growth and fabrication techniques (such as molecular-beam epitaxy and nanolithography) have led to the development of semiconductor devices in which the device response is dominated by ballistic-electron (phase-coherent) transport.[1–5] Such ballistic electrons have been reflected and refracted,[1] focused,[2,3] and interfered[4,5] in a manner analogous to electromagnetic waves in dielectrics. Based on these results, it has been shown analytically, that under the effective-mass approximation, exact, quantitative analogies can be drawn between ballistic (collisionless) electron transport in semiconductors and electromagnetic wave propagation in dielectrics.[6]

These previous analogies were developed both for propagation in the bulk and for propagation past abrupt interfaces between materials.[6] In developing these analogies, the electron wave boundary conditions at an abrupt interface between dissimilar semiconductors were assumed to be the conservation of the electron wave amplitude ψ and the conservation of the product of the inverse effective mass and the normal component of the gradient of the electron wave amplitude, $\nabla\psi\cdot\hat{\mathbf{n}}/m$. The choice of these boundary conditions is equivalent to choosing the Hamiltonian H such that

$$H\psi=\frac{-\hbar^2}{2}\nabla\cdot\left[\frac{\nabla\psi}{m(\mathbf{r})}\right]+V(\mathbf{r})\psi=E\psi\ , \qquad (1)$$

for electron wave propagation in a region of spatially varying effective mass $m(\mathbf{r})$ and spatially varying potential energy $V(\mathbf{r})$, where $\hbar$ is Planck's constant divided by 2π, and E is the total electron energy.[7] This Hamiltonian is probably the most widely used form of the effective-mass Hamiltonian.[7,8] There are, however, other Hermitian forms of the effective-mass Hamiltonian and each results in different boundary conditions.[9,10] von Roos[9] has suggested a Hermitian class of effective-mass Hamiltonian functions. Using this class of functions, Morrow and Brownstein[10] have shown that only those Hamiltonians that lie within a subset of this class of functions have physical meaning when considering the matching of the boundary conditions across an abrupt interface. There is, however, significant disagreement as to the exact form of the Hamiltonian within this class, based on consideration of a number of specific cases.[11–16] The purpose of the present paper, therefore, is to draw a set of exact, quantitative analogies between electromagnetic wave propagation in dielectrics and effective-mass electron wave propagation described by the complete class of Hamiltonians given by Morrow and Brownstein. These analogies will be drawn for propagation in the bulk, propagation past abrupt interfaces, and for propagation within one- and two-dimensionally inhomogeneous materials, and will be valid for whatever form of the general Hamiltonian is ultimately shown to be correct. In addition, these analogies present the specific types of experiments that can be performed to identify the correct form of the effective-mass Hamiltonian.

Morrow and Brownstein[10] demonstrated that, of the general class of Hamiltonians (H) suggest by von Roos,[9] only those that take the form

$$H\psi=\frac{-\hbar^2}{2}(m(\mathbf{r})^{\alpha}\nabla\cdot\{m(\mathbf{r})^{\beta}\nabla[m(\mathbf{r})^{\alpha}\psi]\})+V(\mathbf{r})\psi=E\psi \qquad (2)$$

with the constraint

$$2\alpha+\beta=-1 \qquad (3)$$

have physical meaning, when considering propagation past an abrupt interface between dissimilar semiconductors. Using comparisons of more exact theories and the effective-mass theory, many authors have attempted to deduce the values of α and β, resulting in a wide range of values from $\alpha=-\frac{1}{2}$ and $\beta=0$ (Ref. 11) to $\alpha=0$ and $\beta=-1$ (Refs. 12–14). As Morrow suggests,[11] the determination of the correct values of α and β will doubtlessly depend on experiments. Galbraith and Duggan have used photoluminescence data to shown that $\alpha=0$ and $\beta=-1$ for $GaAs/Ga_{1-x}Ga_xAs$ quantum wells.[15] Similar results have recently been reported for $GaAs/Ga_{1-x}Al_xAs$ quantum wells by Mojahedie and Osinski.[16] However, these results are valid *only* for $GaAs/Ga_{1-x}Al_xAs$ heterostructures.[15] Since the determination of α and β is still an open problem in general, this paper will draw electromagnetic analogies to the general form of the Hamiltonian given in Eq. (2) for all values of α and β. The analogies that are drawn dictate the form experiments must take in order to determine the correct values of α and β.

For the Hamiltonian of Eq. (2), the boundary conditions for an electron wave at an interface are[10]

$$m^{\alpha}\psi \text{ continuous} \tag{4}$$

and

$$m^{\alpha+\beta}\nabla\psi\cdot\hat{\mathbf{n}} \text{ continuous} , \tag{5}$$

where $\hat{\mathbf{n}}$ is the unit vector normal to the interface. Analogously, the boundary conditions for an electromagnetic wave at an interface between two dielectrics require the continuity of the tangential component of the electric field ($\mathcal{E}$) and the continuity of the tangential component of the magnetic field ($\mathcal{H}$) across the interface. Based on this consideration, it is reasonable to look for analogies between $\Phi=m^{\alpha}\psi$ and either $\mathcal{E}$ or $\mathcal{H}$. In the previous work based on Eq. (1), it was demonstrated that ψ (not Φ) was analogous to $\mathcal{E}$ for TE polarization and to $\mathcal{H}$ for TM polarization.[6] The analogies of the present paper will be consistent with these analogies because Eq. (1) is the $\alpha=0$ special case of Eq. (2) for which $\Phi=\psi$.

For bulk propagation in a homogeneous medium, an exact analogy can be drawn between Φ and *both* $\mathcal{E}$ and $\mathcal{H}$. In this case, the Hamiltonian for the electron wave propagation [Eq. (2)] reduces to a Helmholtz equation of the form

$$\nabla^2\Phi=-k^2\Phi , \tag{6}$$

where $k^2=2m(E-V)/\hbar^2$. This wave equation [Eq. (6)] is exactly analogous to the Helmholtz equation for an electromagnetic wave propagating in a homogeneous dielectric of permittivity ϵ and permeability μ, where Φ is replaced by $\mathcal{E}$ for the electric-field equation and by $\mathcal{H}$ for the magnetic-field equation. In the electromagnetic case, $k^2=\omega^2\mu\epsilon$, where ω is the radian frequency of the wave. Since the electron wave Helmholtz equation has exactly the same form as both the electric-field Helmholtz equation and the magnetic-field Helmholtz equation, an exact analogy can be drawn between Φ and *both* $\mathcal{E}$ and $\mathcal{H}$. Using these analogies and the definitions given in Ref. 6, one can define a phase-refractive index for electron waves as

$$n_{\rm ph}^{\rm EW}=m_r^{1/2}(E-V)_r^{1/2} , \tag{7}$$

where $m_r=m/m_{\rm ref}$ is the relative effective mass and $(E-V)_r=(E-V)/(E-V_{\rm ref})$ is the relative kinetic energy, where $m_{\rm ref}$ and $V_{\rm ref}$ are the effective mass and potential energy in a reference region.[6] This electron wave phase-refractive index is analogous to the phase-refractive index for electromagnetic waves $n_{\rm ph}^{\rm EM}=\sqrt{\mu_r\epsilon_r}$, where μ_r is the relative permeability and ϵ_r is the relative permittivity of the dielectric. With these results, phase-propagation effects, such as interference, can be analyzed using standard electromagnetic results where $\mathcal{E}$ (or $\mathcal{H}$) is replaced by Φ and $n_{\rm ph}^{\rm EM}$ is replaced by $n_{\rm ph}^{\rm EW}$. These results are valid for all the Hamiltonians given in Eq. (2).

The above analogies can be extended to describe electron wave propagation past an abrupt interface between materials 1 and 2 with effective masses m_1 and m_2 and potential energies V_1 and V_2, respectively. When a plane wave [the eigensolution to Eq. (6)] is incident upon such an interface, part of the wave is reflected back into region 1 and part of the wave is transmitted (refracted) into region 2. The boundary conditions [Eqs. (4) and (5)] are used to calculate the directions of propagation and the amplitudes of the reflected and transmitted waves. By substituting $\Phi_1=\exp(j\mathbf{k}_{1,i}\cdot\mathbf{r})+r\exp(j\mathbf{k}_{1,r}\cdot\mathbf{r})$ and $\Phi_2=t\exp(j\mathbf{k}_2\cdot\mathbf{r})$ into the boundary conditions [Eqs. (4) and (5)], one finds that

$$\theta_i=\theta_r=\theta_1 , \tag{8}$$

$$n_{\rm ph,1}\sin\theta_1=n_{\rm ph,2}\sin\theta_2 , \tag{9}$$

$$r=\frac{n_{\rm amp,1}\cos\theta_1-n_{\rm amp,2}\cos\theta_2}{n_{\rm amp,1}\cos\theta_1+n_{\rm amp,2}\cos\theta_2} , \tag{10}$$

and

$$t=\frac{2n_{\rm amp,1}\cos\theta_1}{n_{\rm amp,1}\cos\theta_1+n_{\rm amp,2}\cos\theta_2} , \tag{11}$$

where the electron wave amplitude index of refraction is defined as

$$n_{{\rm amp},l}^{\rm EW}=m_{r,l}^{\beta+1/2}(E-V)_{r,l}^{1/2} \tag{12}$$

for region l. These expressions [Eqs. (8)–(11)] are *exactly* the same as the analogous electromagnetic expressions for the reflection and refraction of an electromagnetic wave from an interface between dielectrics 1 and 2 with relative permittivities $\epsilon_{r,1}$ and $\epsilon_{r,2}$ and relative permeabilities $\mu_{r,1}$ and $\mu_{r,2}$ respectively.[6] In the electromagnetic case, Eqs. (10) and (11) give the reflectivity and transmissivity of the electric field for TE polarization and of the magnetic field for TM polarization. Therefore, when considering propagation past an abrupt material interface, Φ is analogous to the electric field for TE polarization and to the magnetic field for TM polarization. In other words, Φ is analogous to the electromagnetic field quantity that is parallel to the interface.[6] In the electromagnetic case, the amplitude index of refraction for region l has one value for TE polarization, $n_{{\rm amp},l}^{\rm TE}=\epsilon_{r,l}^{1/2}/\mu_{r,l}^{1/2}$, and another value for TM polarization, $n_{{\rm amp},l}^{\rm TM}=\mu_{r,l}^{1/2}/\epsilon_{r,l}^{1/2}$.[6] Using the above results for the indices of refraction, one can construct a general set of analogies between electron wave propagation, TE-polarized electromagnetic wave propagation, and TM-polarized electromagnetic wave propagation. This set of analogies is shown in Table I. These analogies, which have been developed for the general form of the effective-mass Hamiltonian given in Eq. (2), are valid for both propagation in the bulk and for propagation past abrupt interfaces between materials. In the case of an abrupt material interface, Eqs. (8)–(11) are valid for electron waves, TE-polarized electromagnetic waves, and TM-polarized electromagnetic waves, where the appropriate indices of refraction are used for each case.

Motivated by the results for abrupt interfaces, one can attempt to draw similar analogies for propagation within materials with general one- and two-dimensional inhomogeneities in effective mass and/or potential energy. Again, the analogy will be drawn between Φ and either $\mathcal{E}$ (for TE polarization) or $\mathcal{H}$ (for TM polarization), where the electromagnetic wave is propagating in a one- or two-dimensionally inhomogeneous dielectric. In this case, TE (TM) polarization is defined as the polarization in which the electric (magnetic) field is polarized normal to the plane containing the gradient of the inhomogeneity. In the case of such an inhomogeneity, the Hamiltonian for the electron wave [Eq. (2)] can be expanded as a wave equation for Φ.

$$\nabla^2\Phi - \left[\frac{\nabla m_r^{-\beta}(\mathbf{r})\cdot\nabla}{m_r^{-\beta}(\mathbf{r})}\right]\Phi + k_0^2 m_r(\mathbf{r})[E-V(\mathbf{r})]_r\Phi = 0 , \tag{13}$$

where $m_r(\mathbf{r}) = m(\mathbf{r})/m_0$ is the varying relative effective mass, $[E-V(\mathbf{r})]_r = [E-V(\mathbf{r})]/(E-V)_0$ is the varying relative kinetic energy, m_0 is the average effective mass, $(E-V)_0$ is the average kinetic energy, and $k_0 = [2m_0(E-V)_0/\hbar^2]^{1/2}$ is the average wave vector of propagation in the medium. This wave equation [Eq. (13)] is exactly analogous to the wave equation for TE propagation in a one- or two-dimensionally inhomogeneous dielectric,

$$\nabla^2\mathcal{E} - \left[\frac{\nabla \mu_r(\mathbf{r})\cdot\nabla}{\mu_r(\mathbf{r})}\right]\mathcal{E} + k_0^2 \mu_r(\mathbf{r})\epsilon_r(\mathbf{r})\mathcal{E} = 0 , \tag{14}$$

where $\mu_r(\mathbf{r}) = \mu(\mathbf{r})/\mu_0$ is the relative permeability modulation, $\epsilon_r(\mathbf{r}) = \epsilon(\mathbf{r})/\epsilon_0$ is the relative permittivity modulation, μ_0 is the average permeability, ϵ_0 is the average permittivity, and $k_0 = (\omega^2\mu_0\epsilon_0)^{1/2}$ is the average wave vector of propagation. By comparison of these wave equations [Eqs. (13) and (14)], one can see that the analogies between electron wave propagation within a one- or two-dimensionally inhomogeneous semiconductor and TE-polarized electromagnetic wave propagation within a one- or two-dimensionally inhomogeneous dielectric are the *same* analogies as those developed for propagation past abrupt material interfaces, which are shown in Table I. As one would expect, a similar analogy exists between electron wave propagation within a one- or two-dimensionally inhomogeneous semiconductor and TM-polarized electromagnetic wave propagation within a one- or two-dimensionally inhomogeneous dielectric,

$$\nabla^2\mathcal{H} - \left[\frac{\nabla \epsilon_r(\mathbf{r})\cdot\nabla}{\epsilon_r(\mathbf{r})}\right]\mathcal{H} + k_0^2 \mu_r(\mathbf{r})\epsilon_r(\mathbf{r})\mathcal{H} = 0 , \tag{15}$$

where the analogies are again given in Table I. Thus, the analogies of Table I are valid for propagation in the bulk, propagation past abrupt material interfaces, and propagation within one- and two-dimensionally inhomogeneous semiconductors. For all of these cases, standard electromagnetic analysis techniques can be used to analyze electron wave effects such as interference, propagation, reflection, refraction, and diffraction, where the analogies of Table I are used.

At this point, one might wonder whether such exact analogies exists for general three-dimensional inhomogeneities. In this case, the analogies do not hold. For general three-dimensional inhomogeneities, decoupled TE and TM polarization cannot be defined. Therefore, one cannot write scalar wave equations [like Eqs. (14) and (15)] for the electric and the magnetic field, but must use the curl equations. Since the vector field quantities are coupled, no exact analogy can be drawn between the vector electromagnetic fields and the scalar electron wave amplitude.

In conclusion, this work has shown that exact, quantitative analogies exist for *all* forms of the general Hamiltonian of Morrow and Brownstein.[10] In addition, these analogies were developed for propagation in the bulk, propagation past abrupt interfaces between materials, and propagation within one- or two-dimensionally inhomogeneous materials. With these analogies, one can analyze a wide class of electron wave effects such as reflection and refraction,[1,2] interference,[4,5] and diffraction[17] using well-understood electromagnetic analysis methods.

An understanding of these electron wave optical effects in semiconductors has become of increasing importance in the past few years. Recent experiments have verified that the electron wave phase index of refraction is proportional to the product of the square root of the kinetic energy[1–3] and the square root of the effective mass.[18,19] It is likely that, in the near future, similar experiments will be performed to verify the dependence of the amplitude index of refraction on kinetic energy and effective mass. Since the form of the amplitude refractive index is linked to the form of the effective-mass Hamiltonian (through $n_{\text{amp}} \propto m^{\beta+1/2}$), experiments that establish the power dependence of the effective mass in the amplitude index of refraction can be used to identify the correct form of the effective-mass Hamiltonian. The recent experiments on transition energies in $GaAs/Ga_{1-x}Al_xAs$

TABLE I. Analogies between effective-mass electron wave propagation and electromagnetic wave propagation in general dielectrics. The previously established constraint $2\alpha+\beta=-1$ applies.

Electron wave EW	Electromagnetic wave TE	TM
$m^{\alpha}\psi$	$\mathcal{E}$	$\mathcal{H}$
m	$\mu^{-1/\beta}$	$\epsilon^{-1/\beta}$
$(E-V)$	$\mu^{1+1/\beta}\epsilon$	$\epsilon^{1+1/\beta}\mu$

quantum wells[15,16] fit this category since the transition energies are strongly dependent on the reflectivity of the barriers (and thus strongly dependent on β).[15] Due to the exact analogies to electromagnetics, it is easy to conceive of other numerous experiments (such as measuring interface reflectivity) to establish this dependence. However, regardless of the results of such experiments, the exact, quantitative analogies established in this paper remain valid. In addition, if the correct form of the Hamiltonian (for material systems other than $GaAs/Ga_{1-x}Al_xAs$) is shown to be other than $\alpha=0$ and $\beta=-1$, the results of previous work based on this assumption (such as Refs. 6 and 17) can be simply modified using Table I, with the analysis methods remaining valid.

This research was supported in part by Grant No, DAAL-03-90-C-0004 from the Joint Services Electronics Program and by Grant No. ECS-9111866 from the National Science Foundation. One of us (G.N.H.) was supported in part by the Office of Naval Research, and one of us (E.N.G.) was supported in part by the National Science Foundation.

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