Theory of Tunneling Across Semiconductor Junctions

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The theory of tunnel diodes is reviewed, and a method developed for calculating the direct tunneling current. The formulation follows Fredkin and Wannier, but since the crystal momentum representation is used, the final details resemble work of Keldysh and of Kane. The method is applicable when the field is not assumed constant throughout the junction region. The calculated transmission probability for an electron between states both sufficiently far from an energy extremum in the Brillouin zone agrees with the usual expressions; but in the case that either the initial or final state nears a band extremum, the transmission probability is found to go continuously to zero.

I. INTRODUCTION: THE TUNNEL DIODE PROBLEM

THE framework of semiconductor tunneling theory was given by Esaki[1] in his original announcement of the tunnel diode. One pictures two fairly homogeneous regions of degenerate-doped semiconductor of opposite type separated by a junction typically 100- to 200-Å wide. The breakdown voltage, at which the current characteristic departs from the form $I=I_0\times[\exp(qV/nkT)-1]$ typifying diffusive transport across the junction, is observed to be slightly positive instead of large and negative. The usual quasiclassical, independent particle theory of semiconductors is presumed adequate for each region by itself. When the current is sufficiently small, the distribution functions $F_R(n,\mathbf{k})$ and $F_L(n,\mathbf{k})$ for the right and left regions are very nearly the equilibrium Fermi distributions. The current density crossing the junction is formally

$$\mathbf{J}_{L\to R}=\sum_n \frac{e}{4\pi^3}\int d^3k \frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}} F_L(n,\mathbf{k}) \times(1-F_R)P_{L\to R}(n,\mathbf{k}) \quad (1.1)$$

plus a similar expression for $\mathbf{J}_{R\to L}$. Here $P_{L\to R}$ is the quantum-mechanical transmission probability that an electron incident on the junction from the left will appear on the right, and the exclusion principle factor $(1-F_R)$ is the statistical probability that the state in which it may appear is unoccupied.[2] Thus the problem of semiconductor tunneling theory reduces to a quantum-mechanical calculation of the transmission probability. The present paper is the first of a series directed at the analysis of this problem.

Section II surveys the semiconductor tunneling calculations made before the discovery of the Esaki diode. Section III discusses the mathematical definition of the probability P which is appropriate for the experimental case of Esaki diodes.

The middle part of the paper contains a number of mathematical preliminaries. Section IV establishes notation and important properties of the complex crystal momentum representation (CMR). Section V mentions a few details of previous tunneling calculations so that their relation to the present calculation will be more explicit. Section VI discusses a "junction potential" operator which replaces the physically less realistic uniform field operator of previous calculations as the source of interband transitions. The explicit representation of this operator in the CMR is one of the important results of this paper.

Finally, in Sec. VII the mathematical approach developed in the preceding sections is worked out in detail for the simple semiconductor model used in nearly all previous calculations. The final formula contains a significant correction which is a direct consequence of the replacement of the completely uniform field by the more realistic junction potential.

It is intended in a future paper to extend the work to other semiconductor models, to consider phonon-assisted tunneling, and to compute directly observable quantities.

II. INTERNAL FIELD EMISSION

In the first quantitative theory of the tunnel diode,[3,4] a transmission probability was found by a simple intuitive adaptation of the theory of "internal field emission" or the Zener effect. The history of this theory will now be reviewed.[5]

In 1934, Zener[6] presented a theory of interband transitions in a one-dimensional semiconductor due to a uniform external field F. By analogy with the WKB method he proposed

$$P=\exp-2\int|k|\,dx, \quad (2.1)$$

where k is the imaginary wave vector associated with a crystal energy in the gap, and the limits of integration are the classical turning points in a deformed band

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[1] L. Esaki, Phys. Rev. **109**, 603 (1958).

[2] In the general case there may be more than one such final state, and the quantity $(1-F_R)P_{L\to R}$ should be summed over these states.

[3] E. O. Kane, J. Appl. Phys. **32**, 83 (1961).

[4] P. J. Price and J. M. Radcliffe, IBM J. Res. Develop. **3**, 364 (1959).

[5] For a complete bibliography up to 1955, see W. Franz, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. XVII.

[6] C. Zener, Proc. Roy. Soc. (London) **145**, 523 (1934).

picture. From the theory of Hill's equation, he deduced that in the almost-free electron case,[7]

$$|k| = ma\pi^{-1}\hbar^{-2}(\tfrac{1}{4}E_g - E^2)^{1/2}, \tag{2.2}$$

where a is the crystal lattice constant, E_g the energy gap, and m is the free-electron mass. The resulting transmission probability is

$$P = \exp - (maE_g^2/4\hbar^2F). \tag{2.3}$$

An alternative form was later presented by Shockley and co-workers.[8] In the almost-free electron case, there is a relation between energy gap and the effective mass m^* at either band edge,

$$am/\hbar = 2\pi(m^*/2E_g)^{1/2}. \tag{2.4}$$

If this relation is used, (2.3) becomes[9]

$$P = \exp - (\pi m^{*1/2}E_g^{3/2}/2\sqrt{2}\hbar F). \tag{2.5}$$

Formula (2.5) has been favored over (2.3) for two reasons: First,[10] the parameters m^*, E_g and F appear to the same powers as the corresponding parameters in the formula for field emission from a potential well. Second,[8] one supposes it is less restricted to the almost-free or small-gap limit.

One difficulty with the Zener formula is that (2.1) is not as firmly based as is the usual WKB method.[11] Houston[12] proposed a somewhat different definition of the interband transition probability for a one-dimensional semiconductor in a uniform external field. He considered the time development of a state which at $t=0$ is an eigenstate of both crystal momentum and band index. The state remains an eigenstate of crystal momentum, and the eigenvalue cycles through the Brillouin zone at the uniform rate $dk/dt = F/\hbar$. Probability amplitude leaks into all other bands, but the rate is greatest for the two adjacent bands. Over the course of a cycle the probability rate is greatest when the k vector is at the band edge. As long as the probability remaining in the initial band is nearly one, the probability per cycle going into another band is nearly independent of time.[13] Houston defined this quantity to be the interband transition probability.

Houston gave without derivation a probability formula with a prefactor of $4\pi^2$ to the exponential (2.3). A later calculation by Homilius[14] of the Houston probability in the almost-free case showed the correct prefactor to be $(\pi/3)^2$. Homilius also[15] preferred the form (2.5) for the exponential. The opinion that this form was the more suitable away from the almost-free limit was given substance by Keldysh,[16] who calculated the Houston probability using properties of complex Bloch waves[17] which were not peculiar to the limit of vanishing energy gap. This established

$$P = \left(\frac{\pi}{3}\right)^2 \exp\left\{-\frac{\pi m^{*1/2}E_g^{3/2}}{2\sqrt{2}\hbar F}\right\} \tag{2.6}$$

as the formaula for "field emission" in a one-dimensional semiconductor. The range of its validity was clarified in a paper by Kane,[18] where the matrix calculation[19] appearing in the almost-free theory was presented in the language of $\mathbf{k}\cdot\mathbf{p}$ perturbation theory. Thus, the formula (2.6) is actually applicable to the case of two bands whose mutual "interaction" is so strong that all other bands may be ignored.

III. THE TRANSMISSION PROBABILITY

Both the Zener and the Houston definitions[20] of interband transition probability are based on the model of a particle in superposed one-dimensional periodic and linear potentials. Fredkin and Wannier[21] proposed adding to the periodic crystal potential not a uniform field but rather a "junction potential."[22] By this is meant a potential which depends only on one position variable and which approaches unequal finite limits as that variable goes to $\pm\infty$. More specifically, let the potential be $V(\mathbf{r}) = V(x)$, where

$$V(-\infty) = 0; \quad V(+\infty) = V_0. \tag{3.1}$$

This model is physically more realistic.

Fredkin and Wannier observed that in their model the transmission probability can be defined as in the theory of free-particle tunneling or of scattering. They considered a stationary state describing a beam incident on

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[7] The expression actually given by Zener is too large by a factor of 2. The error is possibly typographical, because the final expression for the transmission probability is correct.

[8] K. B. McAfee, E. J. Ryder, W. Shockley, and M. Sparks, Phys. Rev. **83**, 650 (1951).

[9] The exponent actually given in Eq. (1) of Ref. 8 is too large by a factor of 2, but in the numerical Eq. (3) of the same paper the exponent is given correctly.

[10] W. Franz, Ergeb. Exakt. Naturw. **27**, 1 (1953).

[11] Cf. the discussion in Sec. V of the actual stationary states and the remark in footnote 20. A mathematical analysis of the WKB method for Bloch electrons is given by P. N. Butcher, D. M. Hum, and E. R. Pike, Proc. Roy. Soc. (London) **A280**, 185 (1964).

[12] W. V. Houston, Phys. Rev. **57**, 184 (1940).

[13] In three dimensions, the path in k space is not cyclic except for special field orientations, and it is not clear how the analysis might rigorously proceed.

[14] J. Homilius, dissertation, Münster (unpublished). J. Homilius and W. Franz, Z. Naturforsch. **9a**, 5 (1954). This work also considers soluble three-dimensional cases.

[15] J. Homilius and W. Franz, Z. Naturforsch. **9a**, 205 (1954).

[16] L. V. Keldysh, Zh. Eksperim. i Teor. Fiz. **33**, 994 (1957) [English transl.: Soviet Phys.—JETP **6**, 763 (1958)]. Due to a computational error Keldysh obtained a prefactor of π^2 instead of $(\pi/3)^2$. The error was corrected in W. Franz, Z. Naturforsch. **14a**, 415 (1959).

[17] Cf. Sec. IV below.

[18] E. O. Kane, J. Phys. Chem. Solids **12**, 181 (1959).

[19] R. Peierls, Ann. Physik **4**, 121, 125 (1930).

[20] The Houston definition actually appeared in a qualitative form at the beginning of Zener's paper, but Zener in fact used the definition (2.1). He did not establish their equivalence, and evidently the two definitions are not equivalent because they lead to different expressions.

[21] D. R. Fredkin and G. H. Wannier, Phys. Rev. **128**, 2054 (1962).

[22] This approach was also implicit in the calculation of Ref. 4.

the junction and analyzed the distribution of the incident probability flux. Outside the junction this stationary state must be a linear combination of Bloch waves. On the left, these waves must be of crystal energy E, to the right $E-V_0$. If $P_{L\to R}(n,\mathbf{k}_0)$ is to be calculated, one imposes the boundary condition that the only Bloch wave with velocity toward the junction is on the left with quantum numbers n and $\mathbf{k}_0$. As will be discussed at the end of Sec. VI, the possibility of more than one outgoing wave on each side cannot be immediately discarded. If the incident wave has unit amplitude and the ith transmitted wave has amplitude T_i, the total transmission probability may be defined as

$$P_{L\to R}(n,\mathbf{k}_0)=\sum_i |T_i|^2 \det[\partial\mathbf{k}_0/\partial\mathbf{k}_i]\,. \quad (3.2)$$

This equation applies only to those $\mathbf{k}_0$ with velocities to the right, i.e., with $\partial E_n(\mathbf{k}_0)/\partial k_x>0$. The transmission probability is *a priori* zero for half of the Brillouin zone. The case of an initial or final velocity parallel to the junction must be studied by letting the velocity component toward the junction approach zero. An example in one dimension appears in Sec. VII.

Since the definition (3.2) ignores interference terms in the probability current, it implicitly assumes that in some sense the electron mean free path is much greater than the junction width, so that an incident packet formed from these scattering states will be able to divide into reflected and transmitted packets before colliding with another electron from the quasiclassical gas on either side of the junction.

It is supposed[1] that a reciprocity law holds, and consequently, the expression for net current can be reduced formally at least to an integral over energy which involves the distribution functions F_R and F_L only as the factor (F_R-F_L). Fredkin and Wannier give a proof for the one-dimensional case.

IV. COMPLEX BAND FORMALISM

This section reviews parts of band theory[23] which will be used later in the paper. The analysis is one-dimensional and possible complications due to band intersection in real k space will not be discussed.

The Hamiltonian H_0 consists of kinetic energy and a potential of period Ω. Its eigenvalue spectrum consists of bands which are doubly degenerate because of time-reversal symmetry. The Bloch eigenfunctions

$$\langle x|nk\rangle=e^{ikx}u_n(k,x) \quad (4.1)$$

are an orthogonal basis for the Hilbert space of one-particle states. Analytic continuation off the real k axis gives Bloch functions which formally satisfy the Schrödinger equation with a complex energy "eigenvalue" but which are not bounded at infinity and hence are outside the space. Since the cell-periodic $u_n(k,x)$ remain bounded, most properties of complex Bloch waves are better studied as properties of the $u_n(k,x)$.

The Bloch functions for one real Brillouin zone, Z, are an orthonormal basis for the one-particle Hilbert space,[24]

$$\langle nk|n'k'\rangle=\sum_G G_0\delta_{nn'}\delta(k'-k+G)$$
$$=\int_{-\infty}^{+\infty} dx e^{i(k'-k)x}u_n(-k,x)u_{n'}(k',x)\,, \quad (4.2)$$

$$\delta(x-x')=\sum_n \int_Z dk G_0^{-1}e^{ik(x-x')}u_n(-k,x')u_n(k,x)\,, \quad (4.3)$$

where G is an arbitrary reciprocal lattice vector and $G_0=2\pi\Omega^{-1}$. The equations defining the crystal momentum representation (CMR) are

$$\langle nk|f\rangle=f_n(k)=\int_{-\infty}^{+\infty} dx e^{-ikx}u_n(-k,x)f(x)\,, \quad (4.4)$$

$$\langle x|f\rangle=f(x)=\sum_n \int_Z dk G_0^{-1}f_n(k)e^{ikx}u_n(k,x)\,. \quad (4.5)$$

For complex k, the state $|nk\rangle$ is strictly speaking outside the Hilbert space, but complex Bloch states can be used in the sense that integrals over the Bloch basis can be deformed off the real k axis. This gives the integrals appearing in field-emission theory an intuitive interpretation.[3] It also simplifies the treatment of states $|f\rangle$ whose distribution $\langle nk|f\rangle$ over the Bloch basis is both discrete and continuous, in particular the Fredkin-Wannier scattering states discussed in Sec. III. Introduction of delta functions or Stieltjes integrals is avoided by defining $\langle nk|f\rangle$ for complex k and prescribing how the inversion contour is to pass around any poles.

The derivation of complex Bloch expansions may be patterned after standard Fourier transform theory. Thus, introduce for any $f(x)$ in the space the auxiliary states

$$\begin{aligned} f_L(x)&=0; \quad x>0 \quad \text{and} \quad f_R(x)=f(x);\ x>0 \\ &=f(x);\ x<0 \qquad\qquad\quad =0; \quad x<0. \end{aligned} \quad (4.6)$$

Then the integral defining $\langle nk|f_L\rangle$ converges for k just above the real axis, that for $\langle nk|f_R\rangle$ just below. The inversion formula (4.5) can be used to recover $f_L(x)$ and $f_R(x)$, provided the contour is deformed off the real axis, over singularities in the case of $\langle nk|f_L\rangle$, under in the case of $\langle nk|f_R\rangle$. Therefore, the representation (4.5) can be used for $f(x)$ itself, with the definition

$$f_n(k)=\langle nk|f_L\rangle+\langle nk|f_R\rangle \quad (4.7)$$

[23] E. I. Blount, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1962), Vol. 13, pp. 305–373.

[24] These formulas assume the cell-periodic functions have been normalized in the unit cell. This normalization is given by Eq. (A.5) or Eq. (A.8) of Appendix A.

and the rule that the inversion contour pass over those singularities of the CMR $f_n(k)$ representing left-hand asymptotic behavior and under the singularities representing right-hand asymptotic behavior.[25]

The complex CMR of the adjoint state may be derived from the complex conjugate of Eq. (4.4),

$$\langle f|nk\rangle=\int_{-\infty}^{+\infty}dx e^{ikx}u_n(k,x)f^*(x)\,. \tag{4.8}$$

The integral for $\langle f_R|nk\rangle$ converges *above* the real axis to $\langle nk^*|f_R\rangle^*$. Thus the prescription for $\langle f|nk\rangle$ is to use $f_n^*(k^*)$ and go around the singularities in the opposite way. This can also be seen directly by taking the complex conjugate of Eq. (4.5):

$$f^*(x)=\langle f|x\rangle=\sum_n\int_{Z^*}dkG_0^{-1}\langle f|nk\rangle\langle nk|x\rangle$$

$$=\sum_n\int_{Z^*}dkG_0^{-1}e^{-ikx}u_n(-k,x)f_n^*(k^*)\,. \tag{4.9}$$

The complex conjugate of Eq. (4.5) can also be written as

$$f^*(x)=\langle x|K|f\rangle=\sum_n\int_Z dkG_0^{-1}\langle x|nk\rangle\langle nk|K|f\rangle$$

$$=\sum_n\int_Z dkG_0^{-1}e^{ikx}u_n(k,x)f_n^*(-k^*)\,, \tag{4.10}$$

where K is the time reversal operator. Hence, the CMR of the time-reversed state is $f_n^*(-k^*)$, and the singularities are treated in the usual way.[26]

V. UNIFORM APPLIED FIELD

This section reviews some details of the one-dimensional quantum mechanics of a particle in superposed periodic and linear potentials, in order to clarify the relation of the field emission calculations discussed in Sec. II to the present theory of Esaki diodes. The stationary states in the periodic potential alone are presumed known. The linear potential operator $-Fx$ can then be divided into in-band and interband parts.[27]

Consider first a Hamiltonian consisting of H_0 plus the in-band part of the linear potential. If at $t=0$ the wave function is the Bloch state $|nk_0\rangle$, then[28]

$$|n,k_0+Ft\rangle\exp-i\times\int_0^t[E_n(k_0+F\tau)-FX_{nn}(k_0+F\tau)]d\tau \tag{5.1}$$

is the state at time t. (In this equation and the remainder of the paper we set $\hbar=1$.) Since this state moves through k space at a uniform rate, the amplitude of the CMR of a stationary state is constant along the real axis. These stationary states will be called "Kane functions" and designated by the letter Q, following Kane.[3,18] Their CMR is[29]

$$\langle nk|Q;E\rangle=Q_n(E,k)=\exp i\int_0^k dk'F^{-1}[E-E_n(k')+FX_{nn}(k')]\,. \tag{5.2}$$

The eigenvalues E for each band form a "Stark ladder" with $\Delta E=F\Omega$. The particular form of the periodic potential affects only the position of each ladder in absolute energy.

In coordinate space the Kane functions are identical in shape but displaced from each other by one cell. The Kane functions for one band form a complete orthonormal basis for that band. Thus they are rather like Wannier functions, which also have uniform probability distribution over the Bloch states of a band and are displaced from each other by one cell. But whereas the Wannier functions are localized to one cell, the Kane functions are localized to the region where $E+Fx$ is an energy in the nth band.[30] In an Appendix, Kane[18] showed how these functions begin to die off going away from this region, but his method breaks down for x halfway into the gap separating the region where $E+Fx$ is in the nth band from the region where it is in the adjacent band. The difficulty in Kane's method stems from the fact that the inversion contour cannot be deformed into the upper half-plane any further than q, the branch point connecting the bands. In itself, this fact suggests that ultimately the Kane functions fall off as $e^{-|qx|}$. Indeed, the proof of such exponential behavior given by Blount[31] for Wannier functions applies to Kane functions as well.

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[25] The choice of a particular Brillouin zone Z is arbitrary; the integrand in (4.5) is periodic and the integral is simply to be taken over one period. The zone boundary is presumed chosen not at a singularity.

[26] This paragraph has described a correspondence between time reversal and reflection across the imaginary axis; the preceding paragraph has described a similar correspondence between taking adjoints and reflecting across the real axis. Both relations are apparent also from the properties of the cell-periodic functions, discussed in Appendix A. Cf. especially Eq. (A.6) and Eq. (A.4).

[27] E. N. Adams, J. Chem. Phys. 21, 2013 (1953). See also Appendix B below.

[28] In Eq. (5.1), $X_{nn}(k)$ is the notation of Adams (Ref. 27). In the notation of Appendix B this quantity is $(nk^*|i\partial/\partial k|nk)$.

[29] The normalization constant in Eq. (5.2) differs from Kane's because Kane chose the reciprocal CMR relations (5.4) and (5.5) differently. Of course this analysis assumes the band does not intersect the adjacent bands in real k space.

[30] These remarks on the x representation of the Kane states may clarify the apparent impossibility (in the CMR) of a simple, rigorous generalization of the Kane states to three dimensions except for a few special lattices and field orientations. Wannier functions of course are easily generalized to three dimensions.

[31] E. I. Blount, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1962), Vol. 13, pp. 331–332.

The situation is not so well understood when the interband part of the linear potential is also included in the Hamiltonian, but some remarks can be made. If a state is $|nk_0\rangle$ at $t=0$, it is always an eigenstate of crystal momentum with eigenvalue k_0+Ft, but it does not remain an eigenstate of band index. If a state is $|Q;n,E\rangle$ at $t=0$, probability amplitude leaks into all other Kane states in general, but presumably most strongly into those of approximately equal eigenvalue and band index.[32] The one-dimensional stationary states again each belong to a "Stark ladder"; there is always a corresponding state shifted in energy by $F\Omega$ and in position by Ω.[33]

VI. THE JUNCTION POTENTIAL OPERATOR

The junction potential operator, V, introduced at the beginning of Sec. III is simple enough in the x representation, but in the CMR it requires some attention. At first, the analysis will be one dimensional. Suppose a state $|f\rangle$ is specified by its CMR, $\langle n'k'|f\rangle=f_{n'}(k')$. Then the CMR relations (4.4) and (4.5) give

$$\langle nk|V|f\rangle=\sum_{n'}\int_Z dk' G_0^{-1} f_{n'}(k')\langle nk|V|n'k'\rangle, \quad (6.1)$$

where

$$\langle nk|V|n'k'\rangle=\int_{-\infty}^{+\infty} dx V(x) e^{i(k'-k)x} u_{n'}(k',x) u_n(-k,x) . \quad (6.2)$$

In Eq. (6.1), the singularities due to $f_{n'}(k')$ are presumed understood, but those due to $\langle nk|V|n'k'\rangle$ must be deduced from Eq. (6.2).

The structure of Eq. (6.2) may be brought out by Fourier analysis. The Fourier transform

$$V(k'')=\int_{-\infty}^{+\infty} dx e^{-ik''x} V(x) \quad (6.3)$$

will have a pole at the origin of residue $-iV_0$. With the boundary conditions (3.1) on the junction potential operator, the inversion contour must pass below the k'' origin. The Fourier series

$$u_n(-k,x)u_{n'}(k',x)=\sum_G C_G e^{iGx} \quad (6.4)$$

has coefficient

$$C_G=\int_\Omega dx \Omega^{-1} e^{-iGx} u_n(-k,x) u_{n'}(k',x) ,$$

which by means of (A.3) and (A.5) of Appendix A may be written

$$C_G=\Omega^{-1}(n, k^*-G|n'k') . \quad (6.5)$$

After substitution of the Fourier expansions in Eq. (6.2), the x integration is done trivially to give $2\pi\delta(k''-k+G+k')$. After the k'' integration Eq. (6.2) becomes

$$\langle nk|V|n'k'\rangle=\sum_G \Omega^{-1}(n, k^*-G|n'k') V(k-G-k') . \quad (6.6)$$

The periodicity of $\langle nk|V|n'k'\rangle$ as a function of k' is manifest in this expansion as a sum of functions identical in shape but shifted by reciprocal lattice vectors. The V factor contributes poles of residue iV_0 at $k-G$. The matrix element does not have these poles for $n\neq n'$ because of the orthonormality of the cell-periodic functions. The k' contour in the $n'=n$ integral must be deformed off the real axis to pass over the pole of the matrix element in the zone of integration, because the k'' contour went under the k'' origin. Boundary conditions on the junction potential different from (3.1) would correspond to a different treatment of the poles in $\langle nk|V|n'k'\rangle$.

Since the CMR of the operator, V is explicitly exhibited in Eq. (6.6), it may be formally divided into in-band part, ϕ and interband part U. Thus the part in the nth band is

$$\langle nk|\phi_n|nk'\rangle=\sum_G \Omega^{-1}(n, k^*-G|nk') V(k-G-k') . \quad (6.7)$$

The generalization to three dimensions is formally trivial. The sum over G becomes a triple series, and the V factor is nonzero only if the real part of $(\mathbf{k}-\mathbf{G}-\mathbf{k}')$ is perpendicular to the junction plane.

Previous tunneling calculations have assumed that $\mathbf{k}_\perp$, the crystal momentum component parallel to the junction plane, is conserved in the tunneling process. From Eq. (6.6) this is evidently not strictly true except for those special geometries where the Houston definition and the Kane functions can be treated rigorously. Consider the tunneling state described in Sec. III, with left-incident wave at $(n,\mathbf{k}_0)$. The junction potential operator mixes in states along a line in k space through $\mathbf{k}_0$ and perpendicular to the junction plane. When reduced to a single zone, this line becomes, in the general case a large number of parallel segments. The transmitted waves can be located in k space by noting where these segments intercept the energy surface $E_{n'}(\mathbf{k})=E_n(\mathbf{k}_0)-V_0$. Thus, the old problem of the nonperiodic path in k space, which plagued the field-emission theory, appears in the present method as the problem of umklapp tunneling processes.

VII. THE TRANSMISSION PROBABILITY FOR THE STANDARD MODEL

This section contains a calculation of the tunneling probability (3.2) for the simple case of a one-dimen-

[32] This situation was considered by Kane (Ref. 18) in his calculation of Eq. (2.6), the Houston probability. He filled a band at $t=0$ by occupying the complete set of Kane states instead of the complete set of Bloch states.

[33] Even in one dimension there is apparently yet no definitive analysis of the form of the eigenfunctions, probably because it is not clear that they have any physical significance. For the view that they do describe observable effects in semiconductor tunneling, see A. G. Chynoweth, G. H. Wannier, R. A. Logan, and D. E. Thomas, Phys. Rev. Letters 5, 57 (1960) and the first two references of that Letter.

sional semiconductor with a small direct gap. The details of the calculation are deliberately made to follow closely the field-emission theory discussed in Secs. II and V.

A. The Completely Reflected State

Let the periodic potential be such that there is a "conduction band" with lower edge at $E=0$ and a gap of width E_g below it, and suppose $V_0>E_g$ as indicated in Fig. 1. When only the in-band part of the junction potential is added to the Hamiltonian, band index may be retained as a quantum number labeling the eigenstates. Crystal momentum no longer commutes with the Hamiltonian, but the eigenstates may be labeled by the k vector of the incident Bloch wave. Thus, $|\beta; nk_0\rangle$ is an eigenstate of $H_0+\phi$ with eigenvalue $E=E_n(k_0)$ for which

$$\beta(x)\sim\langle x|nk_0\rangle+r\langle x|n,-k_0\rangle \tag{7.1}$$

as $|x|\to\infty$ with x of opposite sign from the velocity $v_n(k_0)$.

If $n=c$, the conduction band, then the states of interest are those incident from the left, i.e., those with

$$v_c(k_0)=(\partial/\partial k)E(k_0)>0. \tag{7.2}$$

The CMR wave function $\langle ck|\beta; ck_0\rangle=\beta(k)$ has poles at $\pm k_0$ of residues $i\Omega^{-1}$ and $ir\Omega^{-1}$, respectively, and the inversion contour passes over them.[34] If $E<V_0$, there will be no real k_1 for which

$$E-V_0=E_c(k_1) \tag{7.3}$$

and hence $|r|=1$ by flux conservation. The time-reversed state $K|\beta\rangle$ is then not independent but is $r^*|\beta\rangle$. From Eq. (4.10),

$$\beta(-k^*)=r\beta^*(k)\,. \tag{7.4}$$

But if E is sufficiently large there will be a (conjugate pair of) complex k_1 satisfying (7.3). Then $\beta(k)$ will have a pole at k_1 in the upper half-plane, and $\beta(x)$ will asymptotically die away to the right of the junction like $e^{ik_1x}u_n(k_1,x)$, an unbounded solution of the Schrödinger equation. Even if E is small enough so there is no outgoing pole, $\beta(x)$ is not identically zero once $V(x)$ reaches V_0 because ϕ_n is nonlocal; how fast it dies away depends on how far up the inversion contour can be moved before striking a branch point.

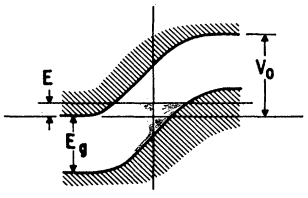

FIG. 1. Deformed band diagram of an Esaki junction.

[34] Cf. the rules derived in Sec. IV above. Strictly speaking, $\beta(k)$ is periodic with period $2\pi/\Omega$ and hence also has poles at $\pm k_0+G$.

According to Eq. (6.7) for ϕ, the CMR Schrödinger equation is

$$[E-E_c(k)]\beta(k)=\int_z dk'(2\pi)^{-1}\beta(k')\times\sum_G(k^*-G\,|\,k')V(k-G-k') \tag{7.5}$$

with the contour passing over $k'=k$.[35] This integral equation shows immediately that as k approaches a branch point, $\beta(k)$ becomes infinite like the normalized cell-periodic function.[36] At $k=\pm k_0$ the equation is finite because the pole in $\beta(k)$ is smoothed out by the zero in $E-E_c(k)$. If there is an outgoing pole, the equation is infinite there, but this infinity may be canceled by rewriting Eq. (7.5) as

$$[E-E_c(k)-V_0]\beta(k)=\int_z dk'(2\pi)^{-1}\beta(k')\times\sum_G(k^*-G|k')V(k-G-k') \tag{7.6}$$

with the contour now passing under $k'=k$.

B. Approximate Solution for $\beta(k)$

Suppose for definiteness that the band gap is at the center of the Brillouin zone. The important part of the function $\beta(k)$ is near the positive imaginary axis below the singularity representing right-hand behavior because this region might be regarded as containing the information about $\beta(x)$ in the junction. For this region the most convenient form of the integral equation for $\beta(k)$ is

$$[E-\tfrac{1}{2}V_0-E_c(k)]\beta(k)=\int_z dk'(2\pi)^{-1}\beta(k')\times\sum_G(k^*-G|k)V(k-G-k')\,, \tag{7.7}$$

in which the principal value is taken at $k'=k$. The situation is shown in Fig. 2.

For the states of interest E will be small enough that $k_0\ll G_0^{-1}$. Furthermore, actual tunnel diode junctions are in the range of 20 to 40 lattice periods wide so that in real directions $V(k)$ is localized to a few percent of the

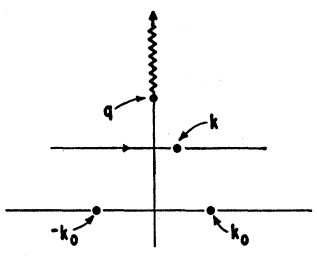

FIG. 2. Singularities of $\beta(k')$ and path of integration for Eq. (7.7).

[35] Henceforth, the band index will be omitted from the round bracket symbol for the inner product of two cell-periodic functions.

[36] This singularity of the cell-periodic functions is discussed in Appendix A. Cf. Eq. (A.5) and Ref. 41.

zone width G_0^{-1}. In these circumstances one may expect the (nonperiodic) solution of

$$[E-\tfrac{1}{2}V_0-E_c(k)]\beta(k) = \int_{-\infty}^{+\infty} dk'(2\pi)^{-1}(k^*|k')V(k-k')\beta(k') \quad (7.8)$$

to be very close to the actual CMR wave function in the important region of k space shown in Fig. 2.

The integral operator in Eq. (7.8) may be expanded as a differential operator by successive partial integrations. The details are presented in Appendix C. If the assumed junction field $F(x)=-dV/dx$ is symmetric about $x=0$, this expansion is

$$\begin{aligned}[E-\tfrac{1}{2}V_0-E_c(k)]\beta(k) &= F_0\langle ck|x|\beta\rangle+\cdots \\ &= F_0[i(\partial/\partial k)+X_{cc}(k)]\beta(k)+R(k)\,, \end{aligned} \quad (7.9)$$

where

$$F_0=-F(0)\,. \quad (7.10)$$

The solution with the remainder $R(k)$ neglected is

$$\beta(k)=N\exp i\int_0^k dk'[E_c(k')-FX_{cc}(k')+\tfrac{1}{2}V_0-E]F_0^{-1}. \quad (7.11)$$

Comparison with Eq. (5.2) shows this CMR wave function to be proportional to the Kane function of eigenvalue E for the linear potential $F_0x+\frac{1}{2}V_0$. The expression (7.11) must be a poor approximation near $\pm k_0$ or q because it does not have the correct singular behavior there.

If the field is constant for the entire width of the junction, the Fourier transform of the junction potential is

$$V(k)=(V_0/ik)\sin(\tfrac{1}{2}kW)/\tfrac{1}{2}kW\,, \quad (7.12)$$

where

$$W=V_0/F_0. \quad (7.13)$$

According to Eq. (C.11) of Appendix C the remainder $R(k)$ on the right side of (7.9) is

$$R(k)=\int_0^\infty dk'2V_0(\pi W)^{-1}\,\mathrm{si}(k'W/2)D_i{}^s(k')\,, \quad (7.14)$$

where si is the standard sine integral and $D_i{}^s$ is defined in (C.7) of Appendix C.

If the approximate solution (7.11) is put into (7.14), it is seen that the approximation is poor when k is less than W^{-1} from the singular points $\pm k_0$ and q. If $|qW|\gg 1$, then there is a strip above the real axis in which (7.11) is a good solution to Eq. (7.8). In x space this may be interpreted as meaning that if the range of the nonlocal potential, ϕ is much less than the width of the junction, from inside the junction the wave function cannot see that the constant field eventually drops to zero.

C. Normalization of the Approximate Solution

The normalization constant N in Eq. (7.11) must be chosen so this approximate solution matches onto that exact solution whose residue at k_0 is $i\Omega^{-1}$. This may be done by putting the approximate solution into the integral equation (7.8) and calculating the residue of the first iterate.

In order to compare directly with previous tunneling papers, the uniform field formula (7.12) is used and X_{cc} taken identically zero. The resulting normalization is

$$N=i[\Omega V_0 I_c(k_0)]^{-1}v_c(k_0)e^{i\epsilon}, \quad (7.15)$$

where

$$\epsilon=\int_0^{k_0} dkF_0^{-1}[E-E_c(k)-\tfrac{1}{2}V_0]\,. \quad (7.16)$$

The quantity $I_c(k_0)$ is given by the expression

$$I_c(k_0)=\int_{-\infty}^{+\infty}\frac{du}{2\pi i}\frac{e^{iu}\sin u}{u^2}(k_0^*|k_0+2uW^{-1})e^{i\Delta}, \quad (7.17)$$

where

$$\Delta=\int_0^u du'2V_0^{-1}[E_c(k_0+2u'W^{-1})-E_c(k_0)] \quad (7.18)$$

and the contour is deformed over the origin.

When $|qW|\gg 1$ it is reasonable to replace $(k_0^*|k_0+2uW^{-1})$ by $(k_0^*|k_0)=1$. Two cases will be considered[37] in approximating the quantity Δ, namely,

$$k_0W\gg 1\,, \quad (7.19a)$$

$$k_0W\ll 1\,. \quad (7.19b)$$

The corresponding approximations are

$$\Delta\approx 2v_c(V_0W)^{-1}u^2;\ k_0W\gg 1\,, \quad (7.20a)$$

$$\Delta\approx 4(3m_c{}^*V_0W^2)^{-1}u^3;\ k_0W\ll 1\,, \quad (7.20b)$$

where v_c is the velocity at k_0 and $m_c{}^*$ is the effective mass at the band edge. For cases of practical interest, a final simplification in (7.17) can be made:

$$e^{iu}\sin u\approx\tfrac{1}{2}i. \quad (7.21)$$

This approximation requires

$$\exp(V_0W/v_c)^{1/2}\gg 1;\ k_0W\gg 1\,, \quad (7.22a)$$

$$\exp(4m_c{}^*V_0W^2)^{1/3}\gg 1;\ k_0W\ll 1\,. \quad (7.22b)$$

With these approximations the integral can be done exactly to give

$$I_c(k_0)\approx -v_c{}^{1/2}(2\pi iV_0W)^{1/2};\ k_0W\gg 1\,, \quad (7.23a)$$

$$I_c(k_0)\approx -3^{1/6}4^{-2/3}\pi^{-1}\Gamma(2/3)(m_c{}^*V_0W^2)^{-1/3};\ k_0W\ll 1\,. \quad (7.23b)$$

[37] Case a of this paper is the only case considered by Fredkin and Wannier in Ref. 21. The condition (7.19) is included in Eq. (58) of that paper.

When these expressions are substituted in (7.15), the normalization constants become

$$|N|^2=(2\pi W v_c V_0^{-1}\Omega^{-2});\ k_0 W\gg 1, \tag{7.24a}$$

$$|N|^2=\alpha k_0 W(2\pi W v_c V_0^{-1}\Omega^{-2});\ k_0 W\ll 1, \tag{7.24b}$$

where

$$\alpha=3.8(m_c^* V_0 W^2)^{-1/3}, \tag{7.25}$$

which is typically close to unity. This means that the penetration of the electron into the junction is significantly decreased when the incident Bloch wavelength is longer than the junction width. This result has not explicitly appeared in previous tunneling theory, although it is perhaps implicit in the work of Fredkin and Wannier.

D. Formula for the Transmitted Amplitude

When the interband part of the junction potential operator is added to the Hamiltonian, the new stationary state $|B;ck_0\rangle$ with incident wave $\langle x|ck_0\rangle$ will, in general, have nonzero CMR, $B_n(k)=\langle nk|B\rangle$, in all bands. The Schrödinger equation is

$$[E-E_n(k)]B_n(k)$$
$$=\langle nk|V|B\rangle=\sum_{n'}\int_z dk'(2\pi)^{-1}B_{n'}(k')$$
$$\times\sum_G\langle n,k^*-G|n'k'\rangle V(k-k'-G)\,, \tag{7.26}$$

corresponding to Eq. (7.5) for $\beta(k)$. In addition to the poles at $B_c(\pm k_0)$, $B_n(k)$ will be singular at $B_v(k_1)$, where $E_v(k_1)=E_c(k_0)-V_0$ and $k_1<0$, as discussed in Sec. VI. The residue at k_1 is $-iT\Omega^{-1}$, and the inversion contour passes under k_1.

One possible approach to the calculation of the transmitted wave amplitude T would be to work directly with Eq. (7.26). All bands other than v and c could be ignored and $\beta(k)$ used as a first approximation to $B_c(k)$. One could next calculate an approximate expression for $B_v(k)$ off the real axis, and finally the residue of its pole at k_1.

Instead the transmitted wave amplitude will be calculated by following the work of Fredkin and Wannier. This will bring out the similarities between the scattering formulation and the older field-emission formulation.

Consider the right-incident eigenstates of $H_0+\phi$ with small positive eigenvalues. These are $|\beta;vk\rangle$ with k small and positive. The CMR, $\langle\beta;vk|vk'\rangle$, as a function of k' will have poles at $+k$ and $-k$ of residues $i\Omega^{-1}$ and $ir^*\Omega^{-1}$, and the k' contour is to pass over these poles. The reflection coefficient r will of course depend on k.

The projection of the left incident eigenstate of H_0+V onto such a right-incident completely reflected state is

$$\langle\beta;vk|B;ck_0\rangle=\int_z dk'G_0^{-1}$$
$$\times\langle\beta;vk|vk'\rangle\langle vk'|B;ck_0\rangle\,, \tag{7.27}$$

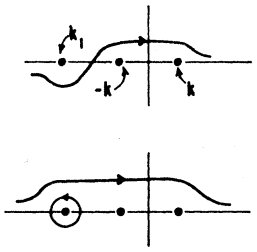

FIG. 3. Alternative contours for the CMR calculation of the projection of a left-incident scattering state onto a right-incident completely reflected state.

The contour for Eq. (7.27) is shown in the upper part of Fig. 3. But this contour is equivalent to the two shown in the lower part of the figure, and the integral around the little circle is $T\langle\beta;vk|vk_1\rangle$. When $k\to -k_1$ this integral has a pole of residue $ir^*T\Omega^{-1}$ and the other term remains finite. Therefore, $\langle\beta;vk|B;ck_0\rangle$ as a function of k has this same residue $ir^*T\Omega^{-1}$ at $-k_1$. From this and the eigenvalue equation for $\langle\beta|$, one has

$$\langle\beta;v,-k_1|E-H_0-\phi|B;ck_0\rangle=-v_v(-k_1)ir^*T\Omega^{-1}, \tag{7.28}$$

which may be rewritten as

$$T=-ir\Omega[v_v(k_1)]^{-1}\langle\beta;v,-k_1|U|B;ck_0\rangle \tag{7.29}$$

by use of the eigenvalue equation for $|B\rangle$.[38] This formula for the transmitted wave amplitude is the analog of the formula for the scattering amplitude in the integral equation treatment of simple potential scattering. In the first Born approximation,

$$T\approx -ir\Omega[v_v(k_1)]^{-1}\langle\beta;v,-k_1|U|\beta;ck_0\rangle\,. \tag{7.30}$$

A formula of this type has been used in several previous tunneling calculations. Fredkin and Wannier[21] discuss the error using (7.30) instead of the exact formula (7.29).

E. The Transmission Probability

In order to use Eq. (7.30) for the transmitted wave amplitude it is necessary to calculate the matrix element

$$M=\langle\beta;v,-k_1|U|\beta;ck_0\rangle\,. \tag{7.31}$$

The procedure of Appendix C for the in-band part of the junction potential can be paralleled for the interband part. The first approximation is

$$M\approx F_0\int_{-\infty}^{+\infty}dkG_0^{-1}\langle\beta;v,-k_1|vk\rangle X_{vc}(k)\langle ck|\beta;ck_0\rangle\,. \tag{7.32}$$

Furthermore, the approximations of Secs. VII.B and VII.C for the conduction band can also be applied to the valence band with the results

$$\langle\beta;v,-k_1|vk\rangle\approx N_v\exp i$$
$$\times\int_0^k dk'[-E_v+FX_{vv}-\tfrac{1}{2}V_0+E]F_0^{-1} \tag{7.33}$$

[38] Equation (7.29) is given without derivation as Eq. (40) by Fredkin and Wannier in Ref. 21.

corresponding to Eq. (7.11) and other expressions identical to Eqs. (7.24) except for the replacement of $v_c(k_0)$ by $v_v(k_1)$.

When Eqs. (7.11) and (7.33) are substituted into Eq. (7.32) and $X_{cc}-X_{vv}$ omitted, as may certainly be done when the crystal has inversion symmetry, the formula for the transition matrix element becomes

$$M\approx F_0\int_{-\infty}^{+\infty} dkG_0^{-1}N_vN_cX_{vc}\exp i\int_0^k dk'(E_c-E_v)F_0^{-1}. \tag{7.34}$$

This integral appears in the Houston[12] formulation of field emission; and in the Keldysh[16] approximation it is

$$M\approx\tfrac{1}{6}F_0\Omega N_vN_ce^{-\frac{1}{2}\lambda}, \tag{7.35}$$

where

$$\lambda=\pi m^{*1/2}E_g^{3/2}/2\sqrt{2}\hbar F_0 \tag{7.36}$$

which is the exponent appearing in Eqs. (2.5) and (2.6). If this expression is used in (7.30), the transmission probability (3.2) becomes

$$P=(1/36)F_0^2\Omega^4|N_v|^2|N_c|^2(v_cv_v)^{-1}e^{-\lambda}. \tag{7.37}$$

The normalization constants are given by Eq. (7.24). If (7.24a) is applicable to both the initial and final states, then P is precisely as in Eq. (7.6).[39] But when either the initial or the final state becomes so close to the band edge that the Bloch wavelength becomes longer than the width of the junction, the transmission probability goes to zero linearly in wave vector with a slope given in Eq. (7.24b).

This interesting result has the satisfying consequence that P is a continuous function of initial wave vector instead of dropping abruptly to zero when the velocity reverses and becomes directed away from the junction. It suggests that the general problem mentioned in Sec. III of velocities parallel to the junction will similarly resolve itself.

A similar situation arises in the problem of a free particle tunneling through a one-dimensional barrier. When either initial or final kinetic energy goes to zero the exact transmission probability goes to zero even though the WKB exponential expression may not; the difficulty is that the usual connection formula breaks down.[40]

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APPENDIX A: CELL-PERIODIC FUNCTIONS FOR COMPLEX CRYSTAL MOMENTUM

The $u_n(k,x)$ appearing in Eq. (2.1) may also be considered as elements of the space $L_2(\Omega)$ of functions defined only for one cell. Rounded brackets $(|)$ will be used for inner products in this space, to distinguish them from inner products $\langle|\rangle$ of one-particle wave functions. For each k the

$$u_n(k,x)=(x|n,k) \tag{A.1}$$

are the eigenfunctions of

$$H_0(k)=e^{-ikx}H_0e^{ikx}. \tag{A.2}$$

Although the Bloch functions themselves are periodic in k space with period $G_0=2\pi/\Omega$, the $|n,k)$ are not. Instead,

$$|n,k+G)=e^{-iGx}|n,k). \tag{A.3}$$

The $|n,k)$ also differ from the Bloch functions in that now analytic continuation off the real k axis does not require extension of the space but rather introduction of non-Hermitian operators $H_0(k)$ whose eigenstates are not mutually orthogonal. Instead there is orthogonality to the eigenstates of the adjoint operator

$$[H_0(k)]^\dagger=H_0(k^*). \tag{A.4}$$

Thus the analytic continuation of the orthonormality relation is

$$(n'k^*|nk)=\int_\Omega dxu_{n'}{}^*(k^*,x)u_n(k,x)=\delta_{nn'}. \tag{A.5}$$

Each cell-periodic function is normalized to unit projection onto the function at k^* in the same band, rather than to unit norm. It can be shown[41] that this requires normalization constant infinite like an inverse fourth root at a complex k where two bands join.

Time reversal K is in the x representation equivalent to complex conjungation. Since $KH_0K^{-1}=H_0$,

$$KH_0(k)K^{-1}=H_0(-k^*). \tag{A.6}$$

Phases may be chosen so that

$$K|nk)=u_n{}^*(k,x)=u_n(-k^*,x)=|n,-k^*). \tag{A.7}$$

The orthonormality relation (A.5) then is also

$$\int_\Omega dxu_{n'}(-k,x)u_n(k,x)=\delta_{nn'}. \tag{A.8}$$

[39] In Ref. 21, Fredkin and Wannier obtain a slightly different formula for the transmission probability in case a. Their exponent λ contains (5/3) instead of $(\pi/2)$ and their prefactor is apparently $(\frac{1}{2}\pi)^2$ instead of $(\frac{1}{3}\pi)^2$. These minor differences may be due to an inconsistency in their method, which is discussed to some extent in Sec. VI of their paper.

[40] This situation is mentioned, for example, by L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1958), p. 175.

[41] A derivation is in the Supplement to Ref. 16. A complete and rigorous proof is in W. Kohn, Phys. Rev. **115**, 809 (1959), Eq. (4.39). The three-dimensional case is discussed on p. 365 of Ref. 23.

APPENDIX B: THE POSITION OPERATOR

Although the position operator x in the CMR is well known, the derivation will be included here so there will be no doubt about how it operates on the *complex* Bloch expansions introduced in Sec. IV.

If the expansion (4.5) is multiplied by some power x^m of the position operator and partially integrated, it becomes

$$x^m f(x)=\int_Z dk G_0^{-1}x^{m-1}e^{ikx}i(\partial/\partial k)[\textstyle\sum_n f_n u_n] -[G_0^{-1}x^{m-1}e^{ikx}\textstyle\sum_n f_n u_n]_Z. \quad \text{(B.1)}$$

If the contour Z can be taken so that $\sum_n f_n u_n$ is differentiable along it, then the integrated term is evaluated only at the endpoints. These cancel by periodicity in k space. When $\sum_n f_n u_n$ is m times differentiable, the expansion becomes

$$x^m f(x)=\int_Z dk G_0^{-1}e^{ikx}(i\partial/\partial k)^m[\textstyle\sum_n f_n u_n]. \quad \text{(B.2)}$$

From this equation the CMR of $x^m|f\rangle$ is easily seen to be

$$\langle jk|x^m|f\rangle=\textstyle\sum_n(jk^*|(i\partial/\partial k)^m f_n(k)|nk). \quad \text{(B.3)}$$

APPENDIX C: EXPANSION OF THE $\beta(k)$ EQUATION

This Appendix gives the details of the expansion of Eq. (7.8). First some auxiliary functions related to the shape of the junction potential must be defined. The Fourier transform (6.3) is separated into real and imaginary parts,

$$V(k)=A(k)+ik^{-1}S(k) \quad \text{(C.1)}$$

which corresponds to separating the junction field into antisymmetric and symmetric parts. Then successive integrals of $A(k)$ and $S(k)$ are defined in the manner of

$$S_1(k)=\int_k^{+\infty} S(k')dk'. \quad \text{(C.2)}$$

The number of times the integration converges at ∞ depends by the Riemann-Lebesgue theorem on the successive differentiability of the assumed junction potential. It is straightforward to establish that at the origin the odd-numbered $A_i(k)$ and $S_i(k)$ have the values

$$A_{2m+1}(0)=\frac{\pi}{i^{2m}}\frac{1}{2m!}\frac{d^{2m}V(0)}{dx^{2m}}, \quad \text{(C.3)}$$

$$S_{2m+1}(0)=\frac{\pi}{i^{2m}}\frac{1}{2m!}\frac{d^{2m}F(0)}{dx^{2m}}, \quad \text{(C.4)}$$

where $F(x)=-dV/dx$ is the junction field.[42]

[42] More accurately, $A_1(0)$ is

$$-\pi\int_{V(x')=0}^{x'=0}[F(x')-F(-x')]dx'.$$

Next some auxiliary functions dependent on the actual solution $\beta(k)$ to (7.8) are defined for a given k as

$$D^S(k')=[(k^*|k+k')\beta(k+k') -(k^*|k-k')\beta(k-k')]/2ik', \quad \text{(C.5)}$$

$$D^A(k')=[(k^*|k+k')\beta(k+k') +(k^*|k-k')\beta(k-k')]/2. \quad \text{(C.6)}$$

The successive derivatives of (C.5) and (C.6) are defined in the manner of

$$D_1{}^S(k')=dD^S/dk'. \quad \text{(C.7)}$$

At the k' origin the odd-numbered derivative functions are zero, since (C.5) and (C.6) are both even. The even-numbered derivative functions have the value

$$D_{2m}{}^S(0)=-\langle ck|x^{2m+1}|\beta\rangle/(2m+1)i^{2m}, \quad \text{(C.8)}$$

$$D_{2m}{}^A(0)=\langle ck|x^{2m}|\beta\rangle/i^{2m}, \quad \text{(C.9)}$$

after use is made of the formula (B.3) of the preceding Appendix for the matrix elements of the position operator.

With these definitions, Eq. (7.8) may be rewritten as

$$[E-\tfrac{1}{2}V_0-E_c(k)]\beta(k)= \int_0^{\infty}[S(k')D^S(k')+A(k')D^A(k')]\pi^{-1}dk'. \quad \text{(C.10)}$$

This equation may be expanded by successive partial integration. The integrated term due to the even-numbered integrations is zero, and the term due to the $(2m+1)$st integration is

$$-\frac{\langle ck|x^{2m+1}|\beta\rangle}{(2m+1)!}\frac{d^{2m}}{dx^{2m}}F(0)+\frac{\langle ck|x^{2m}|\beta\rangle}{2m!}\frac{d^{2m}}{dx^{2m}}V(0).$$

By direct comparison the complete series of these terms is the same as the series that would result from expanding $V(x)$ in a Taylor series and using the known in-band part of powers of the position operator (Appendix B). (The manipulations could be performed on the exact Eq. (7.7), but the complexity seems unwarranted.) Even if the assumed $V(x)$ is analytic along the real axis so that the entire expansion exists, the series is necessarily not convergent. It is, therefore, important to notice the exact remainder term which appears in this derivation.

For example, suppose the junction field is symmetric, so that $A(k)\equiv 0$. Then the result of the first integration of (C.10) is

$$[E-\tfrac{1}{2}V_0-E_c(k)]\beta(k)=-F(0)\langle ck|x|\beta\rangle +\int_0^{\infty}S_1D_1{}^S dk'/\pi. \quad \text{(C.11)}$$

In Sec. VII.B, the second term is neglected as an approximation when k is not near a singularity of $\beta(k)$.