Analytical Models of Interband Tunneling

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Abstract

Analytical formalisms to model interband tunneling, including the Kane method and the WKB approach, are discussed in general. Directions are suggested for how to apply these formalisms to a tunneling device of recent interest, the spiked *pn* junction in GaN, which lacks the simple band structure and uniform fields assumed by conventional models.

1 Introduction

Given the difficulty of creating good ohmic contacts to n-doped GaN, the nitrides community would benefit greatly from alternative structures which allow large currents to flow from p-contacts into n-GaN. One such possibility is "spiked" *pn* junctions in GaN, where the regrowth of the junction interface produces a built-in sheet charge. This sheet charge notches the band diagram, forcing the high electric fields necessary for large tunneling currents. Recent work has derived analytical approximations to the band diagrams of these devices, yet, due to the highly non-uniform fields, simple expressions of the tunneling currents in these devices remain an open problem. Relating the design parameters, eg geometry and doping, of these interfaces to the tunneling current will be vital for rapid modeling if these structures are to find application in LEDs and more.

The initial theoretical studies of interband tunneling began with Keldysh [3] and Kane [2]. In particular, the two-band model of Kane has proven an effective approximation for the study of many direct-gap semiconductors. A major intuitive simplification was introduced by Sze [6], who approximated the problem as a classic tunneling wavefunction through a one-dimensional barrier, neglecting the details of the matrix element and band-structure. Both methods assumed, however, a uniform electric field. Within Sze's picture, this assumption can be relaxed rather simply. Many authors (eg [7], [8]) have since expanded Kane's model as well to non-uniform field, though at the cost of greater mathematical complexity. Given the trade-offs of both Kane's and Sze's approaches, it will be useful to study the application of each model to the non-uniform field profile of the spiked *pn* junction.

2 Sze's WKB method

Given the mathematical ease of Sze's method, it is the more natural place to begin. In a semi-classical, effective mass/envelope function picture of electron transport in a crystal, the state is imagined to be a wavepacket with simultaneously well-defined and smoothly evolving position x and crystal momentum $\hbar k$. The energy E of the tunneling electron is constant, but the bands $E_C(x)$, $E_V(x)$ bend throughout the device. At any position x, one could then determine the electron's energy relative to changing the band edges, and then, from the crystal dispersion relation, compute $k(x)$ for every position.

As the electron enters the classically forbidden region, the x-component of its wavevector passes through zero onto the imaginary axis and the wavepacket decays in amplitude. As the electron exits the region, its wavevector passes back through zero once more and returns to the real axis. Once $k(x)$ is known, the WKB approximation provides a simple expression for the transmission coefficient through a tunneling barrier:

$$T(E) = \exp\left\{-2\int_{x_v}^{x_c} dx|k(x)|\right\}$$

where x_v and x_c are the valence and conduction-side boundaries of the tunnel region.

2.1 Reduction to a scattering problem

To evaluate this integral, $k(x)$ should, in principle, come from the (complex) dispersion relation of the crystal, or some model thereof (eg [1]). In our approach, we will properly evaluate $k(x)$; however, it's worth noting the clever trick which Sze leverages to ignore the details of the dispersion and map the solution onto an introductory-level scattering problem. In explaining this point, we will consider only electrons with no transverse momentum, and we briefly restore the assumption of uniform electric field, $\xi(x) = \xi = E_G/q(x_c - x_v)$.

With the assumption of parabolic bands (both of effective mass m^*) for small k, one can analytically continue the dispersions $E(k) = E_v(x) - \hbar^2k^2/2m^*$, $E(k) = E_c(x) + \hbar^2k^2/2m^*$ onto imaginary k to find valid solutions in the gap. (Note that this only holds near to the respective band edges because of the parabolicity assumption.) So, near x_v, we have $E = E_V(x) + \hbar^2|k|^2/2m^*$. Since, at the start of the tunnel region, $E_V(x_v) = E$, and the slope of E_V is given by ξ, $E_V(x) = E - q\xi(x - x_V)$, and

$$ik(x) = \sqrt{2m^*q\xi(x - x_v)/\hbar^2}$$

The above is formally the same as the classic dispersion of an particle of energy E in a barrier $U(x)$, where $U(x) - E = q\xi(x - x_v)$. Playing the same game near x_c, we find an effective barrier $U(x) - E = q\xi(x_c - x)$. When the electron is deep into the tunneling region, the dispersion is of course more complicated.

Nonetheless, Sze interpolates the simplest algebraic functional form for a barrier $U(x)$ which fits to the above limits. That is the quadratic:

$$U(x) - E = \frac{(E_G/2)^2 - (q\xi x)^2}{E_G}$$

where the zero of x has been implicitly set to the mean of x_c and x_v. In Sze's approximation, the transmission coefficient for interband tunneling is just given by the transmission coefficient of a particle with a familiar parabolic dispersion (and mass m^*) through the above parabolic potential barrier. Conveniently, this coefficient does not even depend on the energy of the tunneling electron (within the WKB approximation, for uniform fields, and ignoring transverse momentum). Note that, if the conduction and valence bands have different effective masses, m^* should be a reduced effective mass; in Sze's convention, $m^* \to m_r^* = 2/(\frac{1}{m_e^*} + \frac{1}{m_h^*})$.

Allowing for transverse momentum can be shown to simply raise the parabolic barrier by $E_\perp = \hbar^2 k_\perp^2 / 2m^*$. Including this effect, and evaluating the WKB integral, we find

$$T(E, E_\perp) = \exp\left\{ -\frac{\pi\sqrt{m^*}(E_G + 2E_\perp)^{3/2}}{2\sqrt{2}q\hbar\xi} \right\}$$

Despite the roughness of the above derivation, Tanaka [8] finds more rigorously that for a two-band model in a uniform field, the exponential dependance of the transmission coefficient is precisely Sze's expression. Given T, one can then sum over the group velocities of all the contributing k-states to find the current.

3 GaN Bandstructure

Sze simplifies the problem by using a parabola with curvature set by the effective mass for the dispersion, but one really should use the material-appropriate imaginary bandstructure in the gap, as shown in 1. In order have a usable form for the bandstructure, we may taken the 4x4 $k \cdot p$ Hamiltonian from [5], and specify it to the $\hat{z}$ direction, which removes most of the off-diagonal matrix elements.

$$H = \begin{pmatrix} E_g + \Delta_{CR} + \frac{\hbar^2 k_z^2}{2m_0} + A_1' k_z^2 & 0 & 0 & iP_1 k_z \\ 0 & \Delta_{CR} + \frac{\hbar^2 k_z^2}{2m_0} + M_2 k_z^2 & 0 & 0 \\ 0 & 0 & \Delta_{CR} + \frac{\hbar^2 k_z^2}{2m_0} + M_2 k_z^2 & 0 \\ -iP_1 k_z & 0 & 0 & \frac{\hbar^2 k_z^2}{2m_0} + L_2' k_z^2 \end{pmatrix}$$

Along this direction, the center 2x2 of the matrix (which form the light and heavy hole bands in real k-space) is uncoupled to the outside 2x2 (which form the conduction and split-off band). So, along the z-axis, the Hamiltonian can

be reduced to an effective two-band model (similar to but more general than [2]).

$$H = \begin{pmatrix} E_g' + \frac{\hbar^2 k_z^2}{2m_e} & iP_1 k_z \\ -iP_1 k_z & \frac{\hbar^2 k_z^2}{2m_h} \end{pmatrix}$$

where

$$\frac{1}{m_e} \equiv \frac{1}{m_0} + \frac{2A_1'}{\hbar^2}, \quad \frac{1}{m_h} \equiv \frac{1}{m_0} + \frac{2L_2'}{\hbar^2}$$

$$E_g' \equiv E_g + \Delta_{CR}, \quad \frac{1}{m_r} \equiv \frac{1}{m_e} + \frac{1}{m_h}$$

and the undefined variables above are expressed in terms of Luttinger-like parameters by [5]. Diagonalizing the above, our band connection in imaginary k-space can be written analytically:

$$k_z(E) = i\sqrt{A(E) + \sqrt{A(E)^2 + B(E)}}$$

$$A(E) = \frac{m_e E g'}{\hbar^2} - \frac{2m_e m_h P_1^2}{\hbar^4} - \frac{m_e m_h E}{m_r \hbar^2}$$

$$B(E) = \frac{4m_e m_h E(E_g' - E)}{\hbar^4}$$

where E is the energy above the valence band-edge. One subtlety worth noting is that, although we have naively found a connection between the split-off (SO) band and the conduction band (CB), the actual continuous connection is between the light-hole (LH) band and conduction band. In our model, the SO crosses through the LH to meet the CB, but, were we to account for spin-orbit coupling, this would be an avoided crossing, so the band which shoots up in imaginary k-space to meet the CB is continuously connected to the LH band, despite its SO character. Since this all happens at small k_z, and what matters is the whole integral of k_z, it's not important to get the avoided crossing correct, so long as we remember that the connection is actually LH-CB.

Much like in Sze's model, adding additional transverse momentum (x-y) increases the imaginary k_z inside the gap, which will exponentially reduce the tunneling current contribution from those states. So, incorporating the contribution from all states with finite transverse momentum requires only an expression that is valid for small transverse momentum k_p. We have not derived a formal expression, but assuming that k_p just broadens the effective band gap by $a(k_p)$ and shifts the k_z up by $b(k_p)$, ie

$$k_z(E, k_p) \approx k_z(E/a(k_p)) + b(k_p)$$

we can fit $a(k_p)$ and $b(k_p)$ as quadratic expressions to the eigenvalues and achieve workable agreement.

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Computationally, this method is straightforward to apply even when the assumptions underlying its simple analytical forms are removed. Starting from

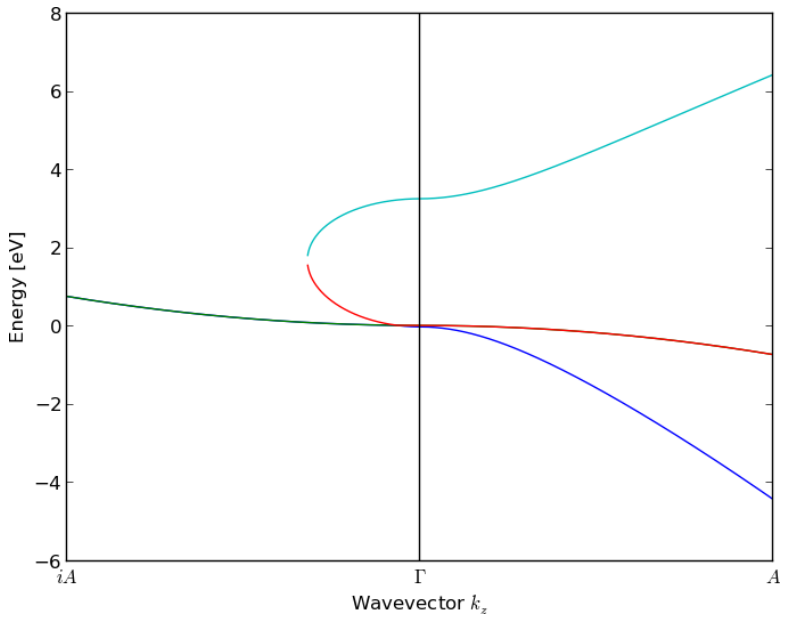

Figure 1: Bandstructure of Gallium Nitride along the $\hat{z}$ direction ($\Gamma \rightarrow A$), continued onto imaginary values of the wavevector (within the $k \cdot p$ approximation, neglecting spin-orbit coupling, using parameters from [5]). In imaginary k-space, the conduction band and light-hole band meet, allowing a particle to "tunnel" continuously between the real bands.

a given band diagram, the procedure is as follows. For each $\vec{k}$ in the valence band that could tunnel to the conduction band (while conserving energy and transverse momentum), find the start and end of the tunnel region (where $k_x = 0$). Then, choosing some determination of k (either Sze's formula, or a band structure model) evaluate 2. Once T is known for all k's, integrate over the band to find a tunnel current.

In the case of uniform fields and parabolic bands/two-band model, the above could be done analytically, since T (above) does not depend on E. However

In preparation for the final presentation, I will be studying the math to approximate this procedure for non-uniform fields and some realistic yet simple band model (likely of the form expressed in [1] or derived from [4]).

4 Kane's model

Whereas Sze's approach could be described as a time-independent WKB method within the effective mass picture of transport, Kane instead applies time-dependent

perturbation theory to the the Wannier equation

$$i\hbar\partial_t\psi_n(r,t) = (E_n^0(k) - e\phi(x))\psi_n(r,t) + \sum_{n\neq n'} W_{n\,n'}\psi_{n'}(r,t)$$

where the effect of the electric field $-\partial_x\phi(x)$ is two-fold. First, by removing translation symmetry, it mixes the k-states within a band, and, secondly, it provides matrix elements $W_{n\neq n'}$ that mix bands together. Kane solves for the wavefunctions with W set to zero, and then applies Fermi's golden rule to determine the transition rate between bands.

In Kane's approach, the Wannier equation is expressed not as above, but rather in the crystal momentum basis. The procedure is the same in principle, though expression in this basis provides an integral which Kane was able to approximate analytically via the method of steepest descent. Nonetheless, use of the crystal momentum basis becomes burdensome for all but the most trivial field profiles (the position operator is represented by a derivative in k-space, so fields that are non-trivial functions of position become higher-order derivatives in the Wannier equation). Recent generalizations of Kane's model to non-uniform fields thus prefer the familiar position representation [8].

4.1 Approach to generalize

All the work discussed involving Kane's method of evaluating the interband tunneling has been within Kane's two-band $k \cdot p$ model of the band structure, which works will for many semiconductors (originally InSb), but less so for III-V's. It would be a useful exercise to try expressions from larger models (ie the 4x4 $k \cdot p$ model which has been fitted to GaN [5]) and see whether the mathematics can still be performed analytically by similar techniques, especially in the context of Tanaka's more general formulation.

5 Summary and Directions

We have discussed two formalisms for determining the transmission coefficients appropriate for direct interband tunneling transitions, and how they might be extended. For the final presentation, I will push both methods in the directions listed toward applicability in the Gallium Nitride spiked pn junction system and compare with experimental data.

References

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