Monte Carlo calculations for metal-semiconductor hot-electron injection via tunnel-junction emission

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We present a detailed description of a scheme to calculate the injection current for metal-semiconductor systems using tunnel-junction electron emission. We employ a Monte Carlo framework for integrating over initial free-electron states in a metallic emitter and use interfacial scattering at the metal-semiconductor interface as an independent parameter. These results have implications for modeling metal-base transistors and ballistic electron emission microscopy and spectroscopy.

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I. INTRODUCTION

A tunnel junction consists of two conductors separated by an insulating potential barrier. When an electrical voltage bias is applied between the two conductors, electrons can convert their potential energy gained by the bias into kinetic energy by tunneling through the thin forbidden zone of the insulator.

Tunnel junctions were studied by Sommerfeld and Bethe and since then have been used with much success for hot-electron spectroscopy. For instance, Giaever et al. studied metallic superconductor gap energies in the early 1960s. More recently, magnetic tunnel junctions (formed between two metallic ferromagnets) have attracted much interest due to their potential as nonvolatile memory elements and hard-drive read heads.

Tunnel junctions have been used for hot-electron injection from metals into semiconductors for decades. First, they were used in solid-state devices to make ultrafast transistors, which mate a tunnel junction to a Schottky diode with a thin base. Later, they served as the basis for a three-terminal microscopy based on the scanning tunneling microscope, known as ballistic electron emission microscopy (BEEM) and its associated spectroscopy (BEES). In this technique, the injected electron current is measured as a function of either the lateral probe position (BEEM) or the tip bias (BEES).

Most theoretical efforts describing metal-semiconductor hot-electron injection via tunnel-junction emission have focused on the latter application of tunnel-junction hot-electron injection (BEES). Many authors have presented theories to explain the features of BEES spectra on various metal-semiconductor systems, including those with heterostructure collectors. In fact, although this paper concerns the Monte Carlo method for this purpose, this scheme has been used numerous times before to model various aspects of this problem: Schowalter and Lee used Monte Carlo to examine hot-electron transport in Au/Si, Ke et al. used it in a simplistic analysis of Au/GaAs, Bauer et al. used it to model Au/GaP and Mg/GaP, and Lee has used a Monte Carlo method to simulate ballistic electron microscopy and attenuation below the Schottky interface. de Andres et al. have also discussed Monte Carlo methods in their review on BEEM. The present paper attempts to give a more detailed treatment of this theory and its finer points than has been previously described.

II. MONTE CARLO FOR BALLISTIC ELECTRONS

The entire process under investigation is essentially a series of two steps, as schematically shown in Fig. 1. The electrons from the emitter (in BEES, a scanning metal tip) first must couple to states in the metal-base layer via tunneling to form a base current. Then, they can couple to states in the semiconductor to form a collector current. The calculation of these currents involves the connection of one momentum state to another by using the principles of energy and parallel momentum conservation in the planar approximation. This is a good assumption for planar devices, such as the metal-base hot-electron transistor, and, in most cases, it is suitable for BEES.

Traditional methods of modeling BEES spectra typically involve the evaluation of complex integrals over initial and final states. The Monte Carlo method replaces numerical methods for solving continuous integrals with random sampling of the complicated integration region of phase space. Monte Carlo’s power in this case is apparent in the fact that only the geometry of k space and knowledge of the connection coefficients are required to calculate values to arbitrary precision. This provides a means to alter the model simply for ad hoc additions, which would otherwise require substantial algorithm revision.

III. TUNNEL JUNCTIONS

For modeling tunnel-junction injection of hot electrons, we have only to sample the space of initial states (from the
emitter), which contribute to the tunneling and transmitted hot-electron collector currents, summing the contributions from each sampling iteration.

The electrons involved in the calculation start their transport in the metal emitter (or STM tip). The simplest model for this metal is the free-electron gas, a model that takes into account only a quadratic dispersion relation and the Pauli exclusion principle. Since this means that

$$\frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) < E_F$$

(1)

for all occupied states at zero temperature, they form a sphere in $k$ space whose radius is determined by the highest filled energy $E_F$ (the Fermi energy), as shown in Fig. 1.

At nonzero temperature $T$, the edge of this sphere is smeared by thermal excitation according to the Fermi-Dirac distribution function,

$$P_{\text{occupation}}(E) = \frac{1}{e^{\beta(E-E_F)} + 1},$$

(2)

where $P_{\text{occupation}}$ is occupation probability and $\beta = 1/(k_B T)$, where $k_B$ is Boltzmann’s constant.

The first step to the Monte Carlo method is to sample a state from among all that have non zero occupation probability. At zero temperature, this applies only to the states within the sphere, but at nonzero temperature, there are partially filled states at every point in $k$ space. However, states far from the Fermi energy have very low occupation probability and so can, with very good approximation, be ignored. Subsequent calculations use a cutoff of $8k_BT$ past $E_F$.

In $k$ space, this corresponds to a sphere with radius

$$k_{\text{high cutoff}}^2 = \frac{2m}{\hbar^2}(E_F + 8/\beta) = \frac{2mE_F}{\hbar^2} \left(1 + \frac{8}{E_F \beta}\right),$$

(3)

and

$$k_{\text{high cutoff}} = \sqrt{\frac{2mE_F}{\hbar^2} \left(1 + \frac{8}{E_F \beta}\right)} = k_F(1 + 4/\beta E_F),$$

(4)

where $k_F$ is the Fermi wave vector.

Our method of choosing an electron state is to randomly pick a point within a cube of side $2k_{\text{high cutoff}}$ centered at $\vec{k} = 0$, until it falls inside a circumscribed sphere of radius $k_{\text{high cutoff}}$. (This is known as the von Neumann rejection method.) Then, we first find the contribution of that state to the base tunneling current (the first step in Fig. 1) by calculating the products of the following:

(i) The thermal occupation probability of the initial (emitter) state.

(ii) The thermal vacancy probability of the final (base) state.

(iii) The incident charge flux on the metal-vacuum interface.

(iv) The tunneling probability.

Then we can calculate the probability that the tunneling electron makes the second step shown in Fig. 1 and contributes to the transmitted collector current. We have already examined component (i). This probability is given by the Fermi-Dirac function. Component (ii) is the probability that the state in the base, which conserves energy and parallel momentum, is not occupied. Since the probability of occupation and vacancy must add to 1, the vacancy probability is given by

$$P_{\text{vacancy}}(E) = 1 - \frac{1}{e^{\beta(E-E_F+eV)} + 1},$$

(5)

where $E$ is the kinetic energy in the emitter and $eV$ is the potential energy gained from biasing the tunnel junction by a voltage $V$.

A. Electron flux

Component (iii), the incident flux, is proportional to the projection of the electron velocity in the direction normal to the interface ($\hbar k_{\perp}/m$); faster moving electrons will impinge on the interface more often and thus have a greater probability of contributing to the tunnel current. We immediately see that the original spherical phase space we want to sample can be reduced to a hemisphere because electrons with velocities having negative components in the emission direction (perpendicular to the interface) can be excluded; they are not incident on the metal-vacuum interface and therefore do not contribute to the base current.

The proportionality constant relating charge flux to perpendicular velocity is the phase-space volume of the sampled state times the electron charge $e$. To calculate this quantity $e\Delta^3k$, we must know how many states there are in the Fermi
sphere. This is determined by the normalization condition
\[
n = \int_{|k|<k_F} \frac{d^3k}{(2\pi)^3}
\]
(at zero temperature).

The real-space electron density \( n \) is an empirically measurable quantity. The Monte Carlo equivalent of this integral is
\[
\sum \Delta^3k = 2N\Delta^3k,
\]
where \( N \) is the sampling number. The factor of 2 is necessary because, although the integral is over the entire sampling sphere, our Monte Carlo sampling is restricted to only the forward-directed hemisphere. Therefore, \( \Delta^3k = n/2N \). For nonzero temperature, we replace \( N \) with the sum of the occupation probabilities,
\[
N_{\text{thermal}} = \sum \frac{1}{e^{\beta(E_E-V_F)}+1}
\]
because we are sampling over a volume that is less dense with electron states.

**B. Tunneling probability**

Component (iv), the tunneling probability, can be a nontrivial exercise in application of the Schrödinger equation if calculated exactly. However, we make use of an important simplification. The tunnel barrier height (for metal-base transistors: oxide conduction band offset; for BEEM/BEEES: the work function of the metal tip) is many \( eV \). The maximum tunneling electron energy (given by the applied bias voltage) is typically around 1 V. The Wentzel-Kramers-Brillouin (WKB) method, an approximation scheme, works well for tunneling processes such as this in which the tunneling energy is far below the barrier height.

The WKB tunneling probability is
\[
P_{\text{WKB}} = e^{-\gamma},
\]
where
\[
\gamma = \frac{1}{\hbar} \int_a^b p(x)dx.
\]
The integration bounds \( a \) and \( b \) are the bounds of the barrier.

For the planar approximation, the applied bias voltage drops evenly across the entire vacuum gap. Therefore, the barrier is a trapezoid, depicted in Fig. 2. We have, then,
\[
\gamma = \frac{1}{\hbar} \int_0^{d_{\text{gap}}} \sqrt{2m\left(-\frac{eV}{d_{\text{gap}}}x + E_E + \phi - E\right)}dx,
\]
where \( d_{\text{gap}} \) is the vacuum gap width, \( V \) is the applied bias voltage, and \( \phi \) is the barrier height. In this planar approximation, \( E \) is the energy determined by the one-dimensional perpendicular component of the momentum \( \hbar^2k_z^2/2m \).

This is a trivial integral; we evaluate it to
\[
\gamma = \frac{2^{3/2}m^{1/2}d_{\text{gap}}}{3\hbar eV}[(E_E + \phi - E)^{3/2} - (E_E + \phi - eV - E)^{3/2}].
\]

**C. Base current summary**

Now we have all the components of the base current contribution of each sampled electron. Since this is a planar theory, the current we calculate is actually a current \( \delta \). We multiply by \( A \), the effective junction area, to convert to a real current.

Our calculation is now to simply evaluate, for states within the sampling sphere, the sum
\[
I_{\text{base}} = eA \frac{\hbar}{m} \frac{n}{2N} \sum k_z P_{\text{occupation}}(E)
\]
\[
\times P_{\text{vacancy}}(E + eV) P_{\text{WKB}}(k_z).
\]
The dominating factor within this sum is the exponentially dependent WKB transmission probability, which is responsible for the sharply peaked energy probability shown in Fig. 3. The parallel momentum distribution is similarly peaked close to \( k_z = 0 \) (Ref. 19).

**D. A simplifying condition**

We can now pause to notice a simplifying condition in our method. For emitter electron states with low energy (for instance, \( E + eV \ll E_F - \beta \)), the vacancy probability for a compatible state in the base is negligibly small. Therefore, we can restrict our sampling space further by ignoring initial
emitter states with energy below a low-energy cutoff; subsequent calculations sample initial states with energy greater than
\[ E_{\text{low cutoff}} = E_F - eV - 8/\beta, \]  
resulting in a cutoff wave vector
\[ k_{\text{low cutoff}}^2 = \frac{2m}{\hbar^2}(E_F - eV - 8/\beta). \]  

By decreasing the phase-space volume of sampled points, our sampling density increases. This greatly improves the accuracy of the calculation because the effect of discretizing phase space is minimized as the limit of continuous sampling is approached. However, our calculation must reflect this limitation of phase-space sampling; \( D \) must now be calculated with an effective sampling
\[ N' = N_{\text{thermal}} + \frac{N}{V_{\text{shell}}}V_{\text{sphere}}. \]  

The first term is the contribution from the electrons that form the base current, with \( E_{\text{low cutoff}} < E < E_{\text{high cutoff}} \). These electrons are in states that form a spherical shell in \( k \) space. The second term accounts for the remaining electrons with \( E_{\text{low cutoff}} < E < E_{\text{high cutoff}} \) which is a sphere. These states have occupation probability very close to unity, and, therefore, we need only count how many of them we would have sampled without the cutoff using the density determined by \( N \), the sampling number.

**E. Results of Monte Carlo tunnel current calculation**

Using this Monte Carlo framework, we have calculated the tunnel-junction current-voltage characteristics using \( 10^6 \) samples in the emitter \( k \) space. This is shown in Fig. 4. We see at least two distinct regimes: at low bias, the current varies linearly with voltage and, at higher bias \( \approx E_F \), the current increases exponentially.\(^{20}\) We can understand this behavior with a simple analysis of our theory.

At low bias, the number of electrons contributing to the base current is small. These electrons originate in states close to the Fermi energy of the emitter, in a thin shell of outer radius \( k_F \) and inner radius of \( \sqrt{2m(E_F-eV)/\hbar} \). Since \( k_{\perp} \) varies little over the thickness of the shell, \( P_{\text{WKB}} \) and the incident flux can be treated to first order as a constant. The dominant effect determining the current change as the bias voltage changes is simply the change in the number of states contributing to the base current. This is determined by the volume of the spherical shell,
\[ \text{Volume} = \frac{4}{3}\pi\left(\frac{\sqrt{2mE_F}}{\hbar}\right)^3 - \frac{1}{3}\left(\frac{3eV}{2E_F}\right)^3. \]  

Therefore, we see that at low bias voltage, the volume (and, hence, the tunnel current) varies, to first order, linearly with bias voltage.

For \( eV > E_F \), every state contributes to the base current, so the above analysis does not apply. The current variation in this so-called Fowler-Nordheim regime is determined by the tunneling probability, which increases exponentially with increasing bias voltage. Even for \( eV < E_F \), the volume of contributing states changes only a small amount as the voltage varies due to the small density of states at low energy, so the exponentially increasing regime begins below the Fermi energy.
travel through the metal base and couple with available states in the semiconductor. Therefore, we must model the following:

(i) Ballistic elastic and inelastic attenuation in the metal base.

(ii) Interfacial elastic scattering at the metal-semiconductor Schottky interface.

(iii) Coupling to semiconductor states.

(iv) Quantum mechanical reflection at the Schottky interface.

A. Attenuation

Component (i) is modeled by using empirical elastic and inelastic mean-free paths for ballistic electrons.\(^{10}\) The mean-free path is a length scale over which the electrons are attenuated by scattering in an average sense. The length scales are determined for different scattering processes; inelastic scattering is, in general, energy dependent because the phase space into which the electron can scatter changes with its initial kinetic energy if energy is not conserved in the scattering process. Higher-energy electrons are scattered more and therefore have shorter mean-free paths than low-energy electrons near the Fermi level.

Combining both elastic and inelastic processes yields


given by

where \(d_{\text{metal}}\) is the thickness of the metal layer.

B. Interfacial scattering

Component (ii) is an addition to the original model of ballistic electron-emission spectroscopy incorporated to take into account empirical observations. It was found that the theoretical spectra fit the experiment observations far better if a portion of the transmitted current were elastically scattered, randomizing the parallel momentum. Therefore, we model this process in the Monte Carlo framework by randomly choosing, with a probability \(SP\), electrons to be scattered via a random reorientation of the wave vector. To assure that this is an elastic process, the norm of the wave vector (proportional to the kinetic energy) is conserved. The algorithm to do this is very similar to our state-sampling algorithm: we choose a random point within a unit sphere and then divide by its norm to make it a unit vector. This unit vector is multiplied by the norm of the original wave vector.

C. Semiconductor conduction band model

We now discuss component (iii). A simple model of the semiconductor states in \(k\) space is the spherical band model. In this model, each of the conduction band valleys have spherical constant-energy surfaces with \(k\)-space radius

\[
R = \frac{\sqrt{2m^*_{\text{DOS}}(E - E_{\text{min}})}}{\hbar},
\]

where \(m^*_{\text{DOS}}\) is the density of states effective mass and \(E_{\text{min}}\) is the conduction band minimum of the conduction valley, with respect to zero energy in the base metal.

To find the semiconductor states compatible with our sampled electron state, we again apply conservation of energy and parallel momentum. The constant energy spheres are constructed and then projected onto the interface Brillouin zone (IBZ), or \(k_i\) plane. A schematic IBZ for GaAs(100), for energy greater than \(E_{\text{min}}\) for the two lowest conduction band valleys \(\Gamma\) and \(L\), is shown in Fig. 5.

If we also project the electron wave vector on this IBZ, it may overlap a projected constant-energy sphere of one of the conduction band minima. If so, it contributes to the collector current because both energy and parallel momentum are conserved. However, its \(k_{\perp}\) necessarily changes due to the band-structure effects. This discontinuity in wave vector causes quantum-mechanical reflection at the metal-semiconductor interface. The electron is transmitted with probability\(^9\)

\[
P_{\text{QM}} = \frac{4k_{\perp}k_{m}}{m_{m}(m_{m}k_{m} + k_{s})^{2}},
\]

where \(m_{m}\) is the effective electron mass in the metal, \(m_{s}\) is the effective electron mass in the semiconductor, and \(k_{m}\) and \(k_{s}\) are the perpendicular components of the electron wave vectors in the metal and semiconductor, respectively. In a “free-electron” metal, \(m_{m}=1\), a common approximation.

The collector current is then the evaluation of the sum

\[
I_{\text{collector}} = e\Lambda \frac{h}{m} \frac{n}{2N'} \sum_{k_{\perp}} k_{\perp} P_{\text{occupation}}(E) \times P_{\text{vacancy}}(E + V) \Gamma_{\text{WB}}(k_{\perp}) P_{\text{attenuation}}(E) \times P_{\text{QM}}(k_{\perp}, E) \int \delta(k_{\perp} - k_{s}) d^{2}k,
\]

where the integral over the \(\delta\) function accounts for parallel momentum conservation at the metal-semiconductor interface.

V. BALLISTIC ELECTRON EMISSION SPECTROSCOPY

In contrast to solid-state tunnel junctions where the geometry (and, hence, the tunnel-current–emitter-voltage relation-
FIG. 6. A 2D projection of the shell-like integration region used in the calculation of the tunnel junction current.

ship) is fixed, the tunneling distance with scanning probe microscopy is variable. In the BEES experiment, as the voltage is varied, the tunnel current is held fixed by increasing the width of the vacuum barrier accordingly via dynamic feedback of tip height. To model this in our simulation, we need to calculate the base current before the collector current is calculated. However, implementing feedback directly in the Monte Carlo algorithm would be very inefficient. Therefore, we accelerate the process of finding the proper vacuum gap by using an integral expression for the tunnel current.

A. Integral expression for tunnel current

We know from the discussion of the zero-temperature tunnel-current theory that in the Monte Carlo formalism,

$$I_{\text{base}} = eA \frac{\hbar}{m} \sum k_{\perp}(E) P_{\text{WKB}}(E) \Delta^3 k.$$

(23)

We convert this sum into an integral by making the standard substitution

$$\Delta^3 k \rightarrow \frac{d^3 k}{(2\pi)^3}$$

(24)

and specifying the bounds of integration.

In analogy to the arguments used before, our integration bounds enclose a half shell in $k$ space with outer radius $k_F$ and inner radius $\sqrt{2m(E_F-eV)/\hbar}$. Figure 6 schematically shows a projection of this region, broken up into two regions labeled I and II. Since the integrand is dependent only on $k_{\perp}$, we can reduce the three-dimensional integral to a one-dimensional integral by a suitable choice of infinitesimal volume element.

Region I is a spherical cap, with $\sqrt{2m(E_F-eV)/\hbar} < k_\perp < k_F$. To exploit the one-dimensional dependence, we use a thin disk as a differential volume element. The radius of this disk $r$ is given by the equation of the circle projected by the Fermi sphere,

$$k_\perp^2 + r^2 = k_F^2,$$

(25)

and because the area of the circle is $A = \pi r^2$, we have for the differential volume element

$$dV = A \cdot dk_{\perp} = \pi(k_F^2 - k_\perp^2)dk_{\perp}.$$

(26)

Region II is the portion of the spherical shell for which $0 < k_\perp < \sqrt{2m(E_F-eV)/\hbar}$. The volume element for this shell is then an annular disk. The area of the annulus is given by the difference between the areas of two concentric disks projected by the Fermi sphere and the inner sphere,

$$A = \pi \left[ (k_F^2) - \left( \frac{2m(E_F-eV)}{\hbar^2} - k_\perp^2 \right) \right] = \frac{2meV}{\hbar^2}$$

(27)

with infinitesimal volume

$$dV = \frac{2meV}{\hbar^2} \cdot dk_{\perp}.$$

(28)

Therefore, we have

$$I_{\text{base}} = \frac{2\hbar}{m(2\pi)^3} \left( \int \frac{2m(E_F-eV)}{\hbar^2} \cdot k_{\perp} e^{-2\gamma} \pi \frac{2meV}{\hbar^2} \cdot dk_{\perp} + \int \frac{k_F}{\sqrt{2m(E_F-eV)/\hbar}} \cdot k_{\perp} e^{-2\gamma} \pi (k_F^2 - k_\perp^2) \cdot dk_{\perp} \right).$$

(29)

Since these two integrals cannot be evaluated analytically, we must use numerical quadrature. We now show the results of this calculation of tunnel current as a function of bias voltage in Fig. 7. Plotted on the same axis is the result of the previously presented Monte Carlo method.

To use these results for vacuum gap compensation to hold the tunnel current constant, we use a bisection algorithm. The effectiveness of this scheme allows the base current to be held to within $10^{-3}$ of the set point in the Monte Carlo simulation with negligible computational overhead.

B. Electron injection results

Due to its relative simplicity, we calculate the BEES for Au/GaAs for voltages where the only contribution is from the $\Gamma$ valley (conduction band minimum). The Schottky barrier used in this calculation is 0.92 eV, and $m^* = 0.067$. These results are shown in Fig. 8.
Notice that the collector current is zero for voltages below the Schottky barrier and increases near quadratically thereafter. It has been claimed that the leading order of the voltage dependence in BEES is actually a $5/2$ power law. From our development of the theory, we can see how this $5/2$ power law arises.

C. Threshold behavior

The three major contributing factors to this power law are conservation of energy, conservation of momentum, and quantum-mechanical scattering. Here we determine the leading order contributions from each in the zero-temperature BEES theory.

1. Conservation of energy

Consider a system where the applied voltage (and thus the potential energy drop) between tip and base is just $\epsilon$ greater than the Schottky barrier height $E_{SB}$. Then, due to conservation of energy across the tunnel barrier,

$$\frac{\hbar^2 k_{tip}^{-2}}{2m} = \frac{\hbar^2 k_{base}^{-2}}{2m} + E_{SB} + \epsilon. \quad (30)$$

The condition for injection of electrons into the semiconductor is

$$\frac{\hbar^2 k_{base}^{-2}}{2m} \geq E_F + E_{SB}. \quad (31)$$

Combining Eqs.(30) and (31), we have

$$\frac{\hbar^2 k_{tip}^{-2}}{2m} \geq E_F - \epsilon. \quad (32)$$

Therefore, at just above threshold, only the electrons in the tip with more kinetic energy than $E_F - \epsilon$ will satisfy the total energy requirement. For these electrons, we have

$$|k_{tip}| \geq \sqrt{\frac{2m}{\hbar^2}(E_F - \epsilon)}. \quad (33)$$

The volume in $k$-space of those electrons that have enough energy to scatter into semiconductor states above the Schottky barrier is then the difference in volumes of two spheres with radii $k_{tip} = k_F$ and $k_{tip} = \sqrt{2m(E_F - \epsilon)/\hbar^2}$, as shown in Fig. 9:

$$\text{Volume} = \frac{4}{3} \pi \left( \sqrt{\frac{2m}{\hbar^2}} \right)^3 \left[ (\sqrt{E_F})^3 - (\sqrt{E_F - \epsilon})^3 \right]. \quad (34)$$

Expanding to first order gives

$$\text{Volume} \approx \frac{4}{3} \pi \left\{ \sqrt{\frac{2m}{\hbar^2}} \right\}^3 \sqrt{E_F \epsilon}. \quad (35)$$

Therefore, the volume of states in $k$ space which contribute to the BEES collector current is proportional to $\epsilon$.

2. Conservation of momentum

Not all electrons with enough energy will couple into semiconductor states. The component of $k$ parallel to the interface plane must be compatible with available states in the semiconductor.

Consider the available states of the $\Gamma$ valley, just above the Schottky barrier. These states form a surface, which projects a disk onto the interface Brillouin zone. Assuming quadratic $E(k)$ dependence, the radius of this disk is proportional to $\sqrt{\epsilon}$.

Since only the electrons with $\vec{k}_0$ inside this disk will enter the semiconductor, the contribution to the BEES collector current above the Schottky barrier will be proportional to the ratio of the areas of the $\Gamma$ valley disk and another disk with radius $k_0$ characteristic of the tunneling process. This situa-
We see that the simulation that most accurately reflects the relative strengths of the thresholds in a clearer way. For comparison, we show the second derivative of the collector current spectra, we show the distribution of the BEES collector current.

VII. CONCLUSION

We have presented a detailed description of Monte Carlo calculations of hot-electron injection via tunnel-junction...
emission for applications to modeling spectroscopies, such as metal-base transistor transfer characteristics and BEES. The method is straightforward but involves many subtleties that drastically increase the effectiveness and accuracy of the calculation. These improvements include reduction of phase space in the emitter Fermi sea to increase the effective sampling density and inclusion of integral methods and minimization to maintain constant tunnel current for BEEM spectroscopy simulation. After examination, this framework allows a simple analysis of the collector current dependence on emitter voltage bias near the Schottky threshold.

Although the computational difficulty of the Monte Carlo method increases when the path through phase space is extended and attaining high accuracy requires dense sampling, this technique is useful even with modest computational facilities. With greater computing power, ad hoc additions can be included to explore more sophisticated uses of hot-electron injection, such as quantum-mechanical transmission through buried heterostructures and interactions with phonons within the collector, leading to energy relaxation and momentum reorientation.

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