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A comparative study of the electron transmission through one-dimensional barriers relevant to field-emission problems

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Abstract

We study the transmission coefficient of one-dimensional barriers that are relevant to field-emission problems. We compare, in particular, the results provided by the simple Jeffreys–Wentzel–Kramers–Brillouin (JWKB) approximation, the continued-fraction technique and the transfer-matrix methodology for the electronic transmission through square, triangular and Schottky–Nordheim barriers (the Schottky–Nordheim barrier is often used in models of field emission from flat metals). For conditions that are typical of field emission (Fermi energy of 10 eV, work function of 4.5 eV and field strength of 5 V nm^{-1}), it is shown that the simple JWKB approximation must be completed by an effective prefactor P_{eff} in order to match the exact quantum-mechanical result. This prefactor takes typical values around 3.4 for square barriers, 1.8 for triangular barriers and 0.84 for the Schottky–Nordheim barrier. For fields F between 1 and 10 V nm^{-1} and for work functions ϕ between 1 and 5 eV, the prefactor P_{eff} to consider in the case of the Schottky–Nordheim barrier actually ranges between 0.28 and 0.98. This study hence demonstrates that the Fowler–Nordheim equation (in its standard form that accounts for the image interaction and that actually relies on the simple JWKB approximation) overestimates the current emitted from a flat metal by a factor that may be of the order of 2–3 for the conditions considered in this work. The study thus confirms Forbes's opinion that this prefactor should be reintegrated in field-emission theories.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Field electron emission is a process by which electrons are emitted from a material because of the application of external fields. It finds applications in the development of flat-panel displays, electronic microscopes, x-ray sources, etc [1]. The process by which this emission occurs, in the cold-emission regime in which the thermal excitation of electrons to energies that are above the apex of the surface barrier can be neglected, turns out to be the quantum-mechanical tunneling of electrons through the surface barrier of the material. In this description, the effect of the external field consists in reducing both the height and the width of the surface barrier, which increases the probability of tunneling and therefore the emission of current.

The first successful model for the emission achieved from a flat metal was proposed by Fowler and Nordheim in 1928 [2]. In their original article, the surface barrier of the emitter only accounted for the external field (thus yielding a triangular barrier). This model was subsequently extended in order to also account for the image interaction [3–5], for band-structure effects [6, 7] and for various other effects [8–10]. The equation $J = at^{-2}\phi^{-1}F^2 \exp[-bv\phi^{3/2}/F]$ that provides the current density J achieved from a flat metal when subject to an external field F is referred to as the standard Fowler–Nordheim equation, although it was actually derived by Murphy and Good [3, 4] as an extension of the work by Fowler and Nordheim in order to include the image interaction. In

this expression, $a = 1.541\,434 \times 10^{-6}$ A eV V^{-2}, $b = 6.830\,890$ eV$^{-3/2}$ V nm^{-1}, v and t are tabulated functions that account for the image interaction and ϕ is the work function of the emitter [11–13].

These models have in common that they apply to a flat emitter. This is actually the reference case. Even when the emitter has a complex three-dimensional structure, it is a common practice to integrate the currents achieved by applying the Fowler–Nordheim equation with the local values of the electric field (this procedure is, however, not valid when the characteristic dimensions of the emitter are below 10 nm) [14]. Except for the original article by Fowler and Nordheim [2], these models also have in common that they depend essentially on the simple Jeffreys [15]–Wentzel [16]–Kramers [17]–Brillouin [18] (JWKB) approximation for evaluating the electronic transmission through the surface barrier [13]. In this approximation, the transmission coefficient is given by $T = \exp[-G]$, where $G = \frac{2\sqrt{2m}}{\hbar}\int_{z_1}^{z_2}[V(z) - E]\,\mathrm{d}z$ (the integration is performed between the classical turning points z_1 and z_2 of the potential barrier $V(z)$ at the normal energy E; m refers to the mass of the electron). We note that the paper by Murphy and Good [3] actually uses on the Kemble formula $T = 1/[1 + \exp(G)]$ for the transmission coefficient [19], but this reduces to the JWKB approximation when $T \ll 1$ as is typically the case in field emission. The derivation by Good and Müller [4] relies explicitly on this JWKB approximation.

It has recently been pointed out by Forbes that an effective prefactor P_{eff} should be included in the transmission coefficient T, which should therefore be expressed as $T = P_{\mathrm{eff}}\exp[-G]$ (this is the Landau and Lifschitz formula) [13, 20, 21]. This prefactor P_{eff} is known analytically for the cases of a square and a triangular barrier. The magnitude of this prefactor P_{eff} is, however, not known for the case of the Schottky–Nordheim barrier (this barrier being that relevant to models of field emission from a flat metal when image effects are included). In a context in which the Fowler–Nordheim equation is widely used by the field-emission community, the author found it useful to apply more exact quantum-mechanical methods in order to establish the accuracy of this JWKB approximation when applied to field-emission problems. This paper will essentially focus on the transmission coefficient that characterizes these different barriers, for given values of the external field F, of the work function ϕ and of the normal energy E (i.e. the electron energy component associated with motion in the direction normal to the emitter surface). Future work will focus on the emission current density actually achieved from a flat emitter.

Different techniques exist for computing the quantum-mechanical transmission through arbitrary one-dimensional barriers. The continued-fraction technique presented by Vigneron and Lambin is one of them [22, 23]. Another technique is provided by the transfer-matrix methodology, which was developed in previous work for the study of three-dimensional problems [24–28]. It is the objective of this paper to compare these two techniques with the simple JWKB approximation. This study aims at establishing the validity of these different schemes and at determining the prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\mathrm{eff}}\exp[-G]$ in order for this approximation to match the results provided by more exact quantum-mechanical techniques. Section 2 presents the different methods used for determining the electronic transmission through one-dimensional barriers. In section 3, these methods are applied successively to square barriers, to triangular barriers and finally to the Schottky–Nordheim barrier. These numerical results are also compared with analytical expressions when available. This work thus settles more quantitatively the accuracy of the JWKB approximation. It also validates the transfer-matrix methodology as a means for getting more exact quantum-mechanical solutions. It finally provides the correction factor P_{eff} to consider when applying the Landau and Lifschitz formula $T = P_{\mathrm{eff}}\exp[-G]$ to field-emission problems.

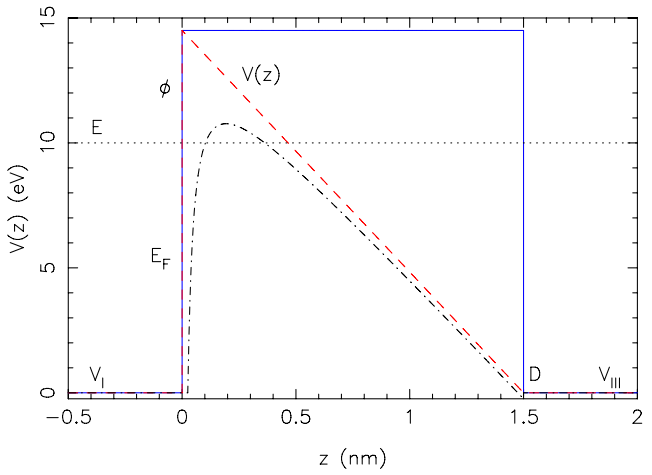

Figure 1. Potential energy for the case of a square barrier (solid), a triangular barrier (dashed) and a Schottky–Nordheim barrier (dot-dashed). The representation corresponds to a Fermi energy E_{F} of 10 eV, a work function ϕ of 4.5 eV and a length D of 1.5 nm for the intermediate Region II.

2. Presentation of different methods for determining numerically the electronic transmission through arbitrary one-dimensional barriers

The problems we consider consist typically of three regions: (i) Region I ($z \leqslant 0$), in which the potential energy has a constant value of V_{I}, (ii) Region II ($0 \leqslant z \leqslant D$), in which the potential energy has an arbitrary dependence $V(z)$ and (iii) Region III ($z \geqslant D$), in which the potential energy has a constant value of V_{III}. Region I corresponds typically to the region that provides the electrons, while Region III corresponds to the region in which the electrons are transmitted. The electron energy E and the potential energies V_{I}, $V(z)$ and V_{III} must be defined with respect to the same reference, whose particular choice is arbitrary and of no significance since we always deal with differences between these different quantities. The usual convention in field-emission theories consists in measuring the energies relative to the bottom of the potential-energy well that represents the emitter. The different barriers considered in this work are depicted in figure 1.

For field-emission problems, we consider that the cathode is subject to an electric field F (we take the field-emission convention that positive values of F correspond to conventional fields that are applied towards the cathode). If D is the length of the intermediate Region II, we actually consider that a bias $V_{\rm ext} = FD$ is established across this region. We can then take $V_{\rm I} = 0$ in Region I, $V(z) = E_{\rm F} + \phi - eFz - \frac{e^2}{16\pi\epsilon_0 z}$ in Region II and $V_{\rm III} = E_{\rm F} + \phi - eV_{\rm ext}$ in Region III (e refers to the absolute value of the charge of the electron, ϵ_0 is the electric constant, $E_{\rm F}$ is the Fermi energy of the metal and ϕ is the work function). For typical metals, we have $E_{\rm F} = 10$ eV and ϕ =4.5 eV.

In order to get the current emitted by the metal, one would need to consider the full set of possible energies, both normal and parallel to the emitter surface. In this paper, one will restrict our attention to particular values of the normal energy E, typically values close to the Fermi energy $E_{\rm F}$. Within the simple Jeffreys–Wentzel–Kramers–Brillouin (JWKB) approximation [15–18], the 'transmission coefficient' of the barrier in Region II is given by $T_{\rm JWKB} = \exp[-G]$, where $G = \frac{2\sqrt{2m}}{\hbar}\int_{z_1}^{z_2}[V(z) - E]\,{\rm d}z$. The points z_1 and z_2 that limit the range of integration correspond to the classical turning points of the barrier at the energy E (we have actually $V(z_1) = E$ and $V(z_2) = E$, with $z_1 < z_2$). This coefficient actually relates the *current densities* in Regions I and III: if the current density associated with an incoming electron in Region I is $J_{\rm in}$, the current density associated with the transmitted electron in Region III is given by $J_{\rm out} = T_{\rm JWKB}J_{\rm in}$ within this approximation. This approximation does not account for interference effects that may occur in the barrier and that are, however, typical of quantum-mechanical problems. Despite this limitation and probably because of its simple analytical expression, this approximation is widely used in applications. In particular, it appears in the model that leads to the standard Fowler–Nordheim equation.

The continued-fraction technique presented by Vigneron and Lambin provides a quantum-mechanical solution for the electronic transmission through arbitrary one-dimensional barriers [22, 23]. Within this scheme, D is split into N segments of length $\Delta z = D/N$. For our problem, one defines $b_N = 2 + \frac{2m\Delta z^2}{\hbar^2}(V_{\rm III} - E)$ and $R_N = \frac{b_N}{2} - {\rm i}\sqrt{1 - b_N^2/4}$. For k going from N to 1, one then computes recursively $b_k = 2 + \frac{2m\Delta z^2}{\hbar^2}[V(k\Delta z) - E]$ and $R_{k-1} = b_k - 1/R_k$. One finally computes $b_0 = 2 + \frac{2m\Delta z^2}{\hbar^2}(V_{\rm I} - E)$ and $R_{-1} = b_0 - 1/R_0$. With $R_0^- = \frac{b_0}{2} - {\rm i}\sqrt{1 - b_0^2/4}$ and $R_0^+ = \frac{b_0}{2} + {\rm i}\sqrt{1 - b_0^2/4}$, the transmission coefficient is finally given by $T_{\rm FC} = 1 - |(R_0^- - R_{-1})/(R_{-1} - R_0^+)|^2$. This 'transmission coefficient' also relates the current densities in Regions I and III. Within the approximation that $\frac{{\rm d}^2\Psi}{{\rm d}z^2} \simeq [\Psi(z - \Delta z) - 2\Psi(z) + \Psi(z + \Delta z)]/\Delta z^2$ for the second derivative of the wavefunction [23], this scheme provides a quantum-mechanical solution for the electronic transmission through an arbitrary barrier $V(z)$ at the energy E.

The third method we consider in this paper is the transfer-matrix technique presented in previous work for the study of three-dimensional problems [24–28]. Let $\Psi_{\rm I}^{\pm} = {\rm e}^{\pm {\rm i}k_{\rm I}z}$ and $\Psi_{\rm III}^{\pm} = {\rm e}^{\pm {\rm i}k_{\rm III}z}$ refer to the solutions of Schrödinger's equation in Regions I and III ($k_{\rm I} = \sqrt{\frac{2m}{\hbar^2}(E - V_{\rm I})}$ and $k_{\rm III} = \sqrt{\frac{2m}{\hbar^2}(E - V_{\rm III})}$). This methodology provides scattering solutions of the form $\Psi^+ \overset{z\leqslant 0}{=} \Psi_{\rm I}^+ + S^{-+}\Psi_{\rm I}^- \overset{z\geqslant D}{=} S^{++}\Psi_{\rm III}^+$, where S^{-+} and S^{++} are the coefficients of, respectively, the reflected and transmitted states for an incident state $\Psi_{\rm I}^+$ in Region I. The way these solutions are established for a one-dimensional barrier is presented with details in the appendix. The 'transmission coefficient' of the potential barrier in Region II is then given by $T_{\rm TM} = \frac{k_{\rm III}}{k_{\rm I}}|S^{++}|^2$. This result relates as previously the *current densities* associated with the incident and transmitted states in, respectively, Regions I and III. In contrast, the factor $|S^{++}|^2$ relates the *probability densities* associated with these incident and transmitted states. Within the approximation that the potential energy $V(z)$ varies in steps in Region II (see the appendix), this methodology provides the *exact* quantum-mechanical result for the transmission coefficient T.

3. Application to square barriers, to triangular barriers and to the Schottky–Nordheim barrier

We compare in this section the JWKB approximation, the continued-fraction technique and the transfer-matrix methodology by considering the results they provide for square barriers, for triangular barriers and finally for the Schottky–Nordheim barrier (this last barrier being that relevant to models of field emission from a flat metal).

3.1. Application to square barriers

In order to compare the results provided by these three techniques with an exact analytical solution, we first consider the case of a square barrier. We take $V_{\rm I} = V_{\rm III} = 0$ eV in Regions I and III. We assume that the barrier in Region II ($0 \leqslant z \leqslant D$) has a height V of 14.5 eV and that the energy E of the incident electron is 10 eV. These values aim at keeping consistent with the Fermi energy $E_{\rm F}$ of 10 eV and with the work function ϕ of 4.5 eV considered later in this paper as representative of typical metals.

For this situation in which $E < V$, the 'transmission coefficient' is given analytically by

$$T_{\rm SB} = \frac{k_{\rm III}}{k_{\rm I}} \times \frac{4}{(1 + \frac{k_{\rm III}}{k_{\rm I}})^2 + [(1 + \frac{k_{\rm III}}{k_{\rm I}})^2 + (\frac{K}{k_{\rm I}} - \frac{k_{\rm III}}{K})^2]\sinh^2(KD)}, \quad (1)$$

where $K = \sqrt{\frac{2m}{\hbar^2}(V - E)}$. The prefactor $\frac{k_{\rm III}}{k_{\rm I}}$ makes this transmission coefficient apply to the *current densities* in Regions I and III (we have as previously $J_{\rm out} = T_{\rm SB}J_{\rm in}$, where $J_{\rm in}$ is the current density associated with the incident electron in Region I and $J_{\rm out}$ is the current density associated with the transmitted electron in Region III).

Figure 2 compares the coefficient transmission T achieved when the energy of the electron ranges from $E_{\rm F} - 3$ eV to $E_{\rm F} +$

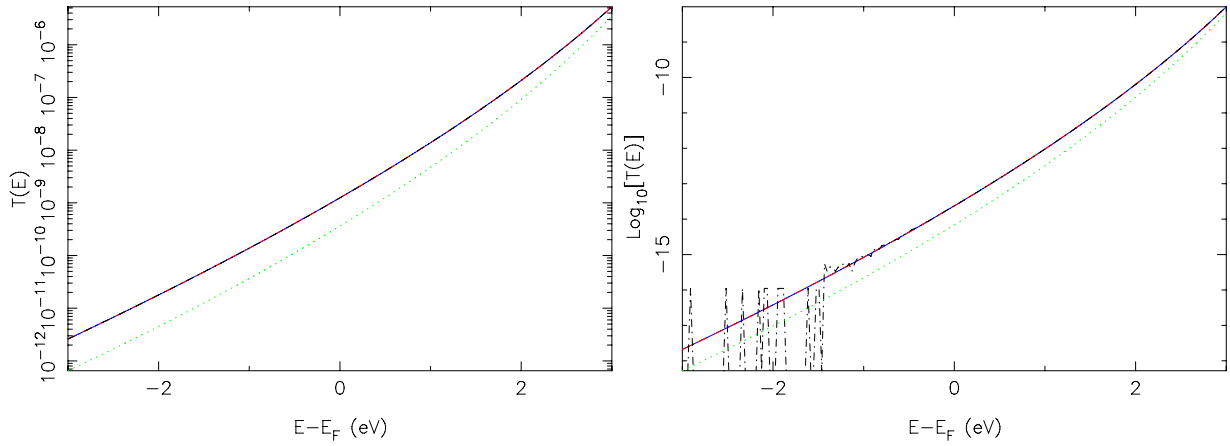

Figure 2. Transmission coefficient T for a square barrier of height $V = 14.5$ eV and of length $D = 1$ nm (left) and 1.5 nm (right). T is computed from its analytical expression (solid), the transfer-matrix technique (dashed), the continued-fraction technique (dot-dashed) and the simple JWKB approximation (dotted). The reference E_F for the energy of the electrons is 10 eV.

3 eV ($E_F = 10$ eV). The figure compares the results achieved for a barrier thickness D of 1 and 1.5 nm. T is calculated from its analytical expression (1), by the transfer-matrix (TM) technique, by the continued-fraction (CF) technique and by the simple JWKB approximation. For $D = 1$ nm, the TM and CF results turn out to be in excellent agreement with each other and with the analytical expression (1). The continued-fraction technique presents, however, numerical instabilities for $D = 1.5$ nm. These instabilities appear systematically when T is less than 10^{-15}. The reason comes from the fact the transmission coefficient $T_{FC} = 1 - |(R_0^- - R_{-1})/(R_{-1} - R_0^+)|^2$ is computed from a representation of the numbers R_{-1}, R_0^- and R_0^+ that is limited to 52 binary digits for their mantissa (this corresponds to a representation with 16 decimal digits). The transfer-matrix technique on the other hand keeps stable over the whole range of conditions. It is for that reason that we use it as a reference when analytical results are not available.

The simple JWKB approximation $T = \exp[-G]$ turns out to provide transmission coefficients that are systematically smaller than the exact quantum-mechanical result by a factor that ranges between 1.5 and 4. The effective prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ in order to match the quantum-mechanical result is represented in figure 3. The results correspond to a length D of 0.5, 1, 1.5 and 2 nm. The prefactor P_{eff} that corresponds to these square barriers is essentially independent of the length D. For $E = 10$ eV, P_{eff} takes the value of 3.424. These conclusions are in excellent agreement with those achieved by Forbes [20]. According to Forbes, the prefactor to consider for the square barrier considered here is given by $P_{\text{eff}}(E) = 16(E - V_I)(V - E)/(V - V_I)^2$ (using our notations and within the assumption that $G \gg 1$). This result is indeed independent of the length D of the barrier. For $E = 10$ eV, the expression given by Forbes provides the value of 3.424, which is in perfect agreement with our numerical result.

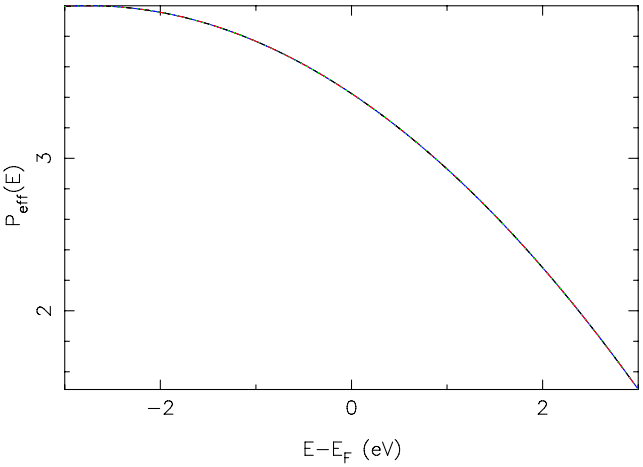

Figure 3. Prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ in order to match the quantum-mechanical result for the transmission through a square barrier with a height V of 14.5 eV and a length D of 0.5 nm (solid), 1 nm (dotted), 1.5 nm (dot-dashed) and 2 nm (dotted). The reference E_F for the energy of the electrons is 10 eV.

3.2. Application to triangular barriers

We now consider a triangular barrier, which is actually the barrier considered in the original paper by Fowler and Nordheim for modeling the emission achieved from a flat metal [2]. We assume that a bias V_{ext} of 1000 V is applied across Region II (this large value aims at reducing the effects of considering that the potential energy in Region III is constant instead of varying with z as in Region II). The slope of the triangular barrier is determined by the field F that characterizes Region II and we have accordingly $D = V_{\text{ext}}/F$ for the length of this region. We take as previously $E_F = 10$ eV and $\phi = 4.5$ eV. We then define $V_I = 0$, $V(z) = E_F + \phi - eFz$ and $V_{III} = E_F + \phi - eV_{\text{ext}}$ for the potential energy in respectively Region I, II and III. The energy E for the electrons is given by $E = E_F$, which corresponds to the Fermi level of Region I.

Figure 4 represents the transmission coefficient T for a triangular barrier, when the field F is 5 and 10 V nm^{-1} (these values are typical in field electron emission). The figure compares the results achieved by the TM methodology, the CF

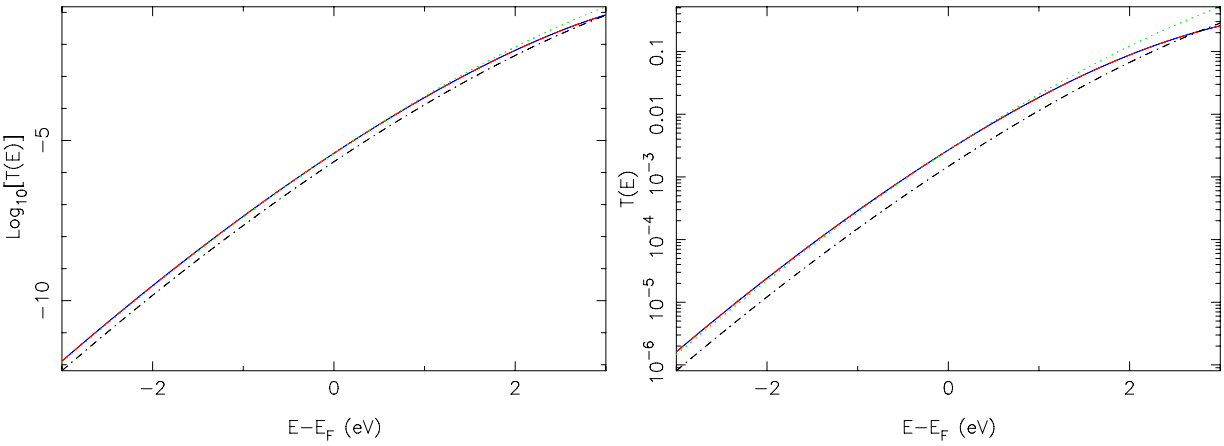

Figure 4. Transmission coefficient T for a triangular barrier corresponding to a field F of 5 V nm^{-1} (left) and 10 V nm^{-1} (right). The Fermi level of the metal in Region I is taken as reference for the normal energy E of the electrons. T is computed from the transfer-matrix technique (solid), the continued-fraction technique (dashed), the simple JWKB approximation $T = \exp[-G]$ (dot-dashed) and the Landau and Lifschitz formula $T = P_{\rm eff}\exp[-G]$ (dotted), where $P_{\rm eff} = 1.839$ (left) and $P_{\rm eff} = 1.820$ (right). The calculations correspond to a Fermi energy of 10 eV and a work function of 4.5 eV.

technique, the simple JWKB approximation $T = \exp[-G]$ and the Landau and Lifschitz formula $T = P_{\rm eff}\exp[-G]$, where $P_{\rm eff}$ is fixed by the value required in order to match the TM result for an electron in Region I with normal energy E equal to the Fermi energy $E_{\rm F}$ ($P_{\rm eff} = 1.839$ for $F = 5$ V nm^{-1} and $P_{\rm eff} = 1.820$ for $F = 10$ V nm^{-1}). These results demonstrate that the JWKB result is smaller than the quantum-mechanical result by a typical factor of 1.8 for an electron with $E = E_{\rm F}$. The approximation that consists in evaluating the transmission coefficient by the formula $T = P_{\rm eff}\exp[-G]$, where $P_{\rm eff}$ is determined for an electron with $E = E_{\rm F}$, actually holds with a good accuracy for energies that do not exceed the Fermi energy by more than 1 eV.

Figure 5 represents the prefactor $P_{\rm eff}$ to use in the Landau and Lifschitz formula $T = P_{\rm eff}\exp[-G]$ in order to match the quantum-mechanical result. $P_{\rm eff}$ is given as a function of the normal energy E and for different values of the electric field F. The prefactor $P_{\rm eff}$ turns out to depend significantly on the electric field F, especially for energies that are closer to the apex of the barrier. The values actually range from 0.9 to 2.0 for the conditions considered. It was established by Fowler and Nordheim [2] that in conditions where $G \gg 1$, $P_{\rm eff}$ should be given by the square root of the value achieved for a square barrier, i.e. $P_{\rm eff}(E) = 4\sqrt{(E - V_{\rm I})(V_{\rm I} + E_{\rm F} + \phi - E)}/(E_{\rm F} + \phi)$ in our notations. For electrons with $E = E_{\rm F}$ ($V_{\rm I} = 0$), this relation indeed provides a value of 1.850, which is in good agreement with the value of 1.848 obtained for $F = 1$ V nm^{-1}. For higher fields, we deviate from the condition $G \gg 1$ for which the previous relation holds. For $F = 10$ V nm^{-1}, we get a prefactor $P_{\rm eff}$ of 1.820, which is smaller (by 1.6%) than the value predicted by this analytical expression.

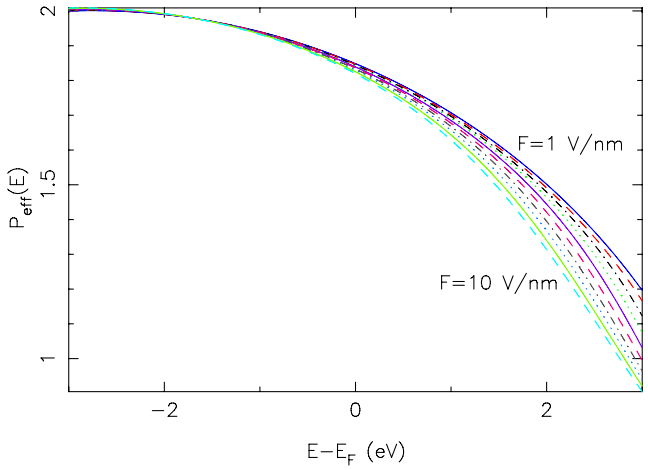

Figure 5. Prefactor $P_{\rm eff}$ to use in the Landau and Lifschitz formula $T = P_{\rm eff}\exp[-G]$ in order to match the quantum-mechanical result for the transmission through a triangular barrier corresponding to a field F that goes from 1 to 10 V nm^{-1} (downwards, by increments of 1 V nm^{-1}). The Fermi level of the metal in Region I is taken as reference for the normal energy E of the electrons. The calculations correspond to a Fermi energy of 10 eV and a work function of 4.5 eV.

3.3. Application to the Schottky–Nordheim barrier

The barrier that is directly relevant to field-emission problems is the Schottky–Nordheim barrier $V(z) = E_{\rm F} + \phi - eFz - \frac{1}{16\pi\epsilon_0}\frac{e^2}{z}$, in which the last term accounts for the image interaction that applies to electrons in Region II. This expression tends to $-\infty$ when $z \to 0$ and the transmission coefficient T actually fails to converge (for physical reasons) if $V(z)$ is not cut. We therefore prevented $V(z)$ from dropping below the reference potential $V_{\rm I}$ of the metal in Region I. This is certainly the most reasonable thing to do in order to model the field-emission barrier and it corresponds indeed to the prescriptions of Murphy and Good [3] and Modinos [11] for this same issue. The way the potential energy in the field region actually connects to that in the metal is probably a delicate issue. Its impact on the field-emission currents is, however, not expected to be significant.

Figure 6 represents the transmission coefficient of the Schottky–Nordheim barrier for a field F of 5 and 10 V nm^{-1}.

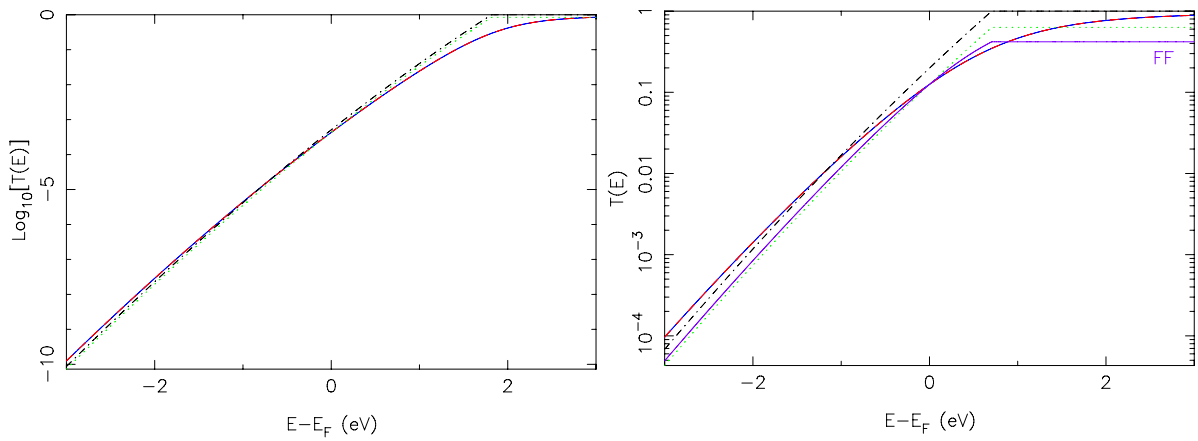

Figure 6. Transmission coefficient T for a Schottky–Nordheim barrier corresponding to a field F of 5 V nm^{-1} (left) and 10 V nm^{-1} (right). The Fermi level of the metal in Region I is taken as reference for the normal energy E of the electrons. T is computed from the transfer-matrix technique (solid), the continued-fraction technique (dashed), the simple JWKB approximation $T = \exp[-G]$ (dot-dashed) and the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ (dotted), where $P_{\text{eff}} = 0.843$ (left) and $P_{\text{eff}} = 0.631$ (right). The figure corresponding to $F = 10$ V nm^{-1} also includes the result achieved using the Fröman and Fröman formula $T = P \exp[-G]/\{1 + P \exp[-G]\}$ (solid, as indicated), where $P = 0.721$. The calculations correspond to a Fermi energy of 10 eV and a work function of 4.5 eV.

We compare the same methods as for the triangular barrier. The results achieved by the transfer-matrix technique and the continued-fraction technique turn out to be in perfect agreement with each other. The JWKB approximation provides a reasonable estimation for the quantum-mechanical result that corresponds to a field F of 5 V nm^{-1} (the prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ is 0.843 for an electron with $E = E_{\text{F}}$ and this formula gives a good account of the quantum-mechanical result for neighboring values of the energy when we keep this value of P_{eff}). For the field F of 10 V nm^{-1}, the results provided by the JWKB approximation and the Landau and Lifschitz formula do not follow the quantum-mechanical result (the prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ is 0.631 for $E = E_{\text{F}}$ and this formula does not account accurately for the transmission achieved for other values of the normal energy if P_{eff} is not adapted). The JWKB approximation and the Landau and Lifschitz formula actually fail because the normal energy E is sufficiently close to the apex of the barrier. The Fröman and Fröman formula $T = P \exp[-G]/\{1 + P \exp[-G]\}$ is better suited, in principle, to describe these situations in which the transmission coefficient T is close to 1 [20, 29]. The result obtained using the Fröman and Fröman formula with $P = 0.721$ is also included in figure 6 (this value of P is that required in order to match the transfer-matrix result for $E = E_{\text{F}}$; it is different from the effective prefactor $P_{\text{eff}} = 0.631$ to use in the Landau and Lifschitz formula). The results achieved with the Fröman and Fröman formula are indeed closer to the exact result than those achieved with the Landau and Lifschitz formula. They deviate, however, immediately from the exact result as soon as the energy changes from the value for which the prefactor P is calculated.

Since the JWKB approximation is so widely used, even at the level of fundamental theories relevant to field emission [4, 3], it is useful to represent the correction factor P_{eff} to consider in the Landau and Lifschitz formula

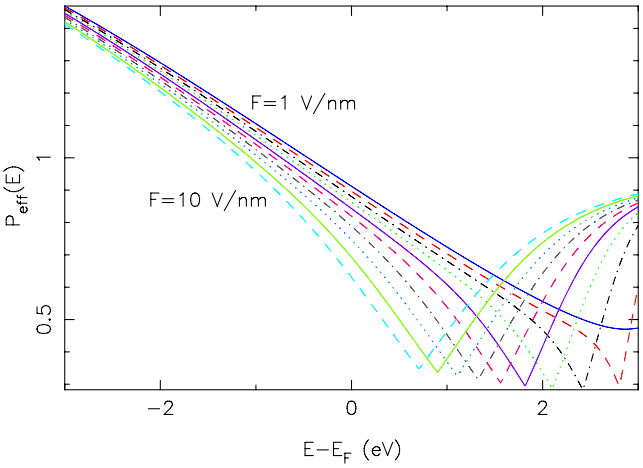

Figure 7. Prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ in order to match the quantum-mechanical result for the transmission through a Schottky–Nordheim barrier corresponding to a field F that goes from 1 to 10 V nm^{-1} (downwards, by increments of 1 V nm^{-1}). The Fermi level of the metal in Region I is taken as reference for the normal energy E of the electrons. The calculations correspond to a Fermi energy of 10 eV and a work function of 4.5 eV.

$T = P_{\text{eff}} \exp[-G]$ in order to match the exact quantum-mechanical result. This is done in figure 7, where we represented the prefactor P_{eff} to consider in order to get this exact result. The results are presented as a function of the energy E, for different values of the electric field F. The different curves show an inflection at the critical field $F_{\text{crit}} = \frac{4\pi\epsilon_0\phi^2}{e^3}$ for which the apex of the barrier corresponds to the Fermi level of the metal in Region I (this inflection also appears for the prefactor P that is relevant to the Fröman and Fröman formula). For fields F that are higher than this critical value, the electrons at the Fermi level of the metal can actually escape to the vacuum by ballistic motion over the barrier. A realistic

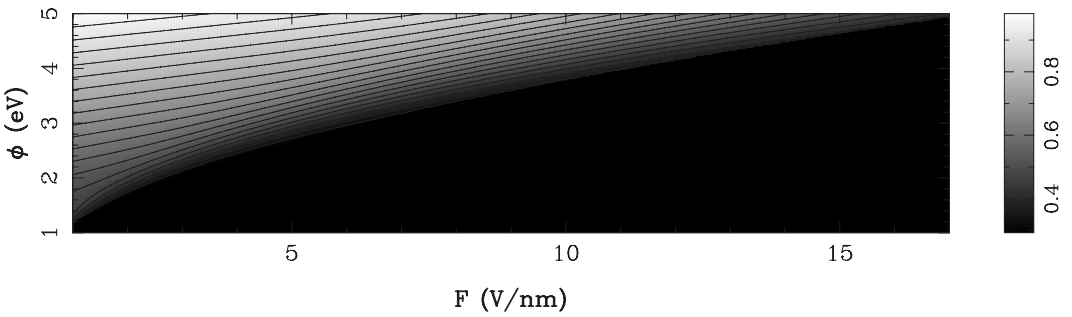

Figure 8. Prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ in order to match the quantum-mechanical result for the transmission through a Schottky–Nordheim barrier when the energy of the electrons corresponds to the Fermi level of the metal. The results are represented as a function of the field F and work function ϕ. The representation is restricted to fields F that keep below $F_{\text{crit}} = \frac{4\pi\epsilon_0\phi^2}{e^3}$. The calculations correspond to a Fermi energy of 10 eV.

Table 1. Coefficients a_{ij} of the polynomial adjustment $P_{\text{eff}} = \sum_{i=0}^{6}\sum_{j=0}^{5} a_{ij} X^i Y^j$ for the effective prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ for the transmission through a Schottky–Nordheim barrier. In this expression, $X = F - 1.7$ with F the external field in V nm^{-1} and $Y = \phi - 4.9$ with ϕ the work function in eV. This expression is restricted to $F < \frac{4\pi\epsilon_0\phi^2}{e^3}$, 1 V nm$^{-1} \leqslant F \leqslant 10$ V nm^{-1} and 3 eV $\leqslant \phi \leqslant 5$ eV.

a_{ij}	$j=0$	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$
$i=0$	$9.600\,74 \times 10^{-1}$	$1.432\,71 \times 10^{-1}$	$-1.113\,97 \times 10^{-2}$	$-7.261\,57 \times 10^{-3}$	$-5.431\,73 \times 10^{-3}$	$-1.341\,12 \times 10^{-3}$
$i=1$	$-1.375\,16 \times 10^{-2}$	$4.568\,18 \times 10^{-3}$	$2.991\,42 \times 10^{-4}$	$2.324\,42 \times 10^{-3}$	$-8.739\,25 \times 10^{-5}$	$-4.623\,23 \times 10^{-4}$
$i=2$	$-2.687\,18 \times 10^{-4}$	$1.653\,58 \times 10^{-3}$	$1.054\,99 \times 10^{-2}$	$2.802\,02 \times 10^{-2}$	$2.141\,83 \times 10^{-2}$	$4.869\,67 \times 10^{-3}$
$i=3$	$-1.486\,93 \times 10^{-4}$	$-8.513\,43 \times 10^{-4}$	$-6.353\,84 \times 10^{-3}$	$-1.688\,41 \times 10^{-2}$	$-1.006\,88 \times 10^{-2}$	$-1.461\,63 \times 10^{-3}$
$i=4$	$7.255\,32 \times 10^{-5}$	$1.084\,26 \times 10^{-4}$	$1.052\,75 \times 10^{-3}$	$3.014\,34 \times 10^{-3}$	$9.569\,29 \times 10^{-4}$	$-7.639\,32 \times 10^{-5}$
$i=5$	$-1.456\,05 \times 10^{-5}$	$9.632\,13 \times 10^{-6}$	$-6.266\,99 \times 10^{-5}$	$-1.926\,09 \times 10^{-4}$	$3.814\,86 \times 10^{-5}$	$3.430\,46 \times 10^{-5}$
$i=6$	$7.573\,64 \times 10^{-7}$	$-1.249\,26 \times 10^{-6}$	$1.093\,99 \times 10^{-6}$	$3.655\,80 \times 10^{-6}$	$-4.604\,76 \times 10^{-6}$	$-1.208\,45 \times 10^{-6}$

metal would not sustain this regime and the conditions that are relevant to practical problems correspond to $F < F_{\text{crit}}$. In this range of field values, P_{eff} ranges between 0.283 and 1.469 for the conditions considered. These values are smaller than those corresponding to the triangular barrier. They are indicative of the accuracy one can expect from field-emission models that rely on the simple JWKB approximation.

The results presented so far correspond to a work function ϕ of 4.5 eV for the metal in Region I. In figure 8, we represented the prefactor P_{eff} to consider in the Landau and Lifschitz formula when we let the work function take values between 1 and 5 eV. The representation is restricted to fields F that keep below $F_{\text{crit}} = \frac{4\pi\epsilon_0\phi^2}{e^3}$. These P_{eff} values are those to consider for electrons with $E = E_{\text{F}}$ in order get the exact quantum-mechanical result for their transmission $T = P_{\text{eff}} \exp[-G]$ through the surface barrier. The normal energy at which these P_{eff} values are calculated corresponds to that usually considered in field-emission theories. Within the approximation that the same P_{eff} could be used for the different energies that contribute to the field-emission current, figure 8 would actually represent the correction factor to consider in order to get a more exact emission current (the standard Fowler–Nordheim equation relies indeed on the simple JWKB approximation; if J_{FN} is the current density predicted by this equation, $P_{\text{eff}} J_{\text{FN}}$ would represent a better approximation for this current density). As demonstrated in this paper, P_{eff}, however, depends on the energy E and further work will be necessary to determine the correction factor to consider with the Fowler–Nordheim equation. For the conditions considered in figure 8, P_{eff} ranges between 0.283 and 0.984. It thus shows that the currents predicted by models that rely on the simple JWKB approximation overestimate the currents one would obtain from a flat metal by a factor that can reach values of the order of 2–3 for fields F that are close to the critical value F_{crit}. This issue will be addressed in more detail in future work.

Before concluding this work, we provide a polynomial adjustment for the data represented in figure 8. The effective prefactor P_{eff} to use in the Landau and Lifschitz formula $T = P_{\text{eff}} \exp[-G]$ can be well represented by the best-fit expression $P_{\text{eff}} = \sum_{i=0}^{6}\sum_{j=0}^{5} a_{ij} X^i Y^j$, where $X = F - 1.7$ with F the external field in V nm^{-1} and $Y = \phi - 4.9$ with ϕ the work function in eV. The coefficients a_{ij} of this adjustment are given in table 1. This expression applies for external fields F that keep below $F_{\text{crit}} = \frac{4\pi\epsilon_0\phi^2}{e^3}$. It is subject to the restrictions 1 V nm$^{-1} \leqslant F \leqslant 10$ V nm^{-1} and 3 eV $\leqslant \phi \leqslant 5$ eV. For this range of parameters, this best-fit expression of the results provided by the TM methodology is characterized by a maximum absolute error of 2.2×10^{-3} and by a mean error of 2.1×10^{-4}. The reader can contact the author to obtain polynomial expressions that cover a wider range of parameters or to obtain the TM routines used for these calculations.

4. Conclusion

This paper addressed the quantum-mechanical calculations of the electronic transmission through one-dimensional barriers that are relevant to field-emission problems. We compared

in particular the results provided by the simple JWKB approximation, the continued-fraction technique and the transfer-matrix methodology for the case of square, triangular and Schottky–Nordheim barriers. The study confirmed that the simple JWKB approximation must be completed by an effective prefactor P_{eff} (thus yielding the Landau and Lifschitz expression $T = P_{\text{eff}} \exp[-G]$ for the transmission coefficient) in order to match the exact quantum-mechanical result. For conditions that are typical of field emission (Fermi energy of 10 eV, work function of 4.5 eV and external field of 5 V nm^{-1} for the triangular and Schottky–Nordheim barriers), we have typically $P_{\text{eff}} \simeq 3.4$ for square barriers, $P_{\text{eff}} \simeq 1.8$ for triangular barriers and $P_{\text{eff}} \simeq 0.84$ for the Schottky–Nordheim barrier (these values are relevant to electrons with a normal energy equal to the Fermi energy). With fields F that range between 1 and 10 V nm^{-1}, P_{eff} actually takes values between 0.91 and 0.63 for the Schottky–Nordheim barrier. If we allow the work function ϕ to take values between 1 and 5 eV, P_{eff} then ranges between 0.28 and 0.98. As observed by Forbes, the prefactor P_{eff} is smaller for 'smooth' (ideal) barriers than for 'sharp' (nonideal) barriers [13, 20]. For a given type of barrier and as long as F does not exceed the critical field F_{crit} that cancels the surface barrier for the normal energy E considered, we observe that P_{eff} decreases with the normal energy E of the electrons and with the strength of the field F. It increases with the work function ϕ. The smaller values achieved for P_{eff} actually correspond to the conditions for which $T \simeq 0.5$, which corresponds to $F \simeq F_{\text{crit}}$. These results are important in the context of field emission since applications will actually tend to these conditions (they correspond indeed to higher emissions of current). The prediction of these currents often relies on the Fowler–Nordheim equation, which depends in turn on the JWKB approximation. This study, however, shows that this approximation deviates from the exact quantum-mechanical result by a factor P_{eff} that can be as small as 0.28 for the conditions considered. The Fowler–Nordheim equation thus overestimates the current achieved from a flat metal by a factor that can reach values of the order of 2–3 for fields F that are close to their critical value. This may affect any analysis of field-emission data that is based on the Fowler–Nordheim equation. This issue will be addressed in more detail in future work.

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Appendix. The transfer-matrix methodology for the electronic transmission through arbitrary one-dimensional barriers

Let V_{I} and V_{III} refer to the constant values of the potential energy in Region I ($z \leqslant 0$) and Region III ($z \geqslant D$). The intermediate Region II ($0 \leqslant z \leqslant D$) is characterized by an arbitrary potential energy $V(z)$ and we seek to determine the transmission of electrons with an energy E through this barrier.

The boundary states in Regions I and III are given, respectively, by $\Psi_{\text{I}}^{\pm} = \mathrm{e}^{\pm \mathrm{i} k_{\text{I}} z}$ and $\Psi_{\text{III}}^{\pm} = \mathrm{e}^{\pm \mathrm{i} k_{\text{III}} z}$, where $k_{\text{I}} = \sqrt{\frac{2m}{\hbar^2}(E - V_{\text{I}})}$ and $k_{\text{III}} = \sqrt{\frac{2m}{\hbar^2}(E - V_{\text{III}})}$. The transfer-matrix methodology actually provides scattering solutions of the form

$$\Psi^{+} \overset{z \leqslant 0}{=} \Psi_{\text{I}}^{+} + S^{-+}\Psi_{\text{I}}^{-} \overset{z \geqslant D}{=} S^{++}\Psi_{\text{III}}^{+}, \tag{A.1}$$

$$\Psi^{-} \overset{z \leqslant 0}{=} S^{--}\Psi_{\text{I}}^{+} \overset{z \geqslant D}{=} \Psi_{\text{III}}^{-} + S^{+-}\Psi_{\text{III}}^{+}, \tag{A.2}$$

which correspond to incident states in, respectively, Regions I and Region III. The first solution, equation (A.1), is actually that required in order to compute the transmission coefficients considered in this paper. The presentation will therefore focus on the establishment of this solution only.

The procedure for getting a scattering solution of the form (A.1) actually consists in establishing an intermediate solution

$$\Psi \overset{z \leqslant 0}{=} A_{\text{I}}\Psi_{\text{I}}^{+} + B_{\text{I}}\Psi_{\text{I}}^{-} \overset{z \geqslant D}{=} \Psi_{\text{III}}^{+}, \tag{A.3}$$

which corresponds to an outgoing state Ψ_{III}^{+} in Region III. In order to determine the coefficients A_{I} and B_{I}, one needs to propagate the values of $\Psi(z)$ and $\frac{\mathrm{d}\Psi(z)}{\mathrm{d}z}$ from $z = D$, where these values are perfectly defined, to $z = 0$. This is done by assuming that the potential energy $V(z)$ in Region II varies in steps between $z = 0$ and D. If we take N steps of length $\Delta x = D/N$ and define $z_l = l\Delta z$, we actually assume that the potential energy takes the constant value $V_l = [V(z_{l-1}) + V(z_l)]/2$ in each step $z_{l-1} \leqslant z \leqslant z_l$, where $l = 1, \ldots, N$.

The wavefunction $\Psi(z)$ and its derivative $\frac{\mathrm{d}\Psi(z)}{\mathrm{d}z}$ take then in each step the analytical expressions

$$\Psi(z) = A_l \mathrm{e}^{\mathrm{i}k_l z} + B_l \mathrm{e}^{-\mathrm{i}k_l z}, \tag{A.4}$$

$$\frac{\mathrm{d}\Psi(z)}{\mathrm{d}z} = \mathrm{i}k_l(A_l \mathrm{e}^{\mathrm{i}k_l z} - B_l \mathrm{e}^{-\mathrm{i}k_l z}), \tag{A.5}$$

where $k_l = \sqrt{\frac{2m}{\hbar^2}(E - V_l)}$ (to keep concise, we allow at this point k_l to be imaginary if $E < V_l$). If the values of $\Psi(z_l)$ and $\frac{\mathrm{d}\Psi(z_l)}{\mathrm{d}z}$ are known, one has

$$A_l = \frac{1}{2}\mathrm{e}^{-\mathrm{i}k_l z_l}\left[\Psi(z_l) + \frac{1}{\mathrm{i}k_l}\frac{\mathrm{d}\Psi(z_l)}{\mathrm{d}z}\right], \tag{A.6}$$

$$B_l = \frac{1}{2}\mathrm{e}^{\mathrm{i}k_l z_l}\left[\Psi(z_l) - \frac{1}{\mathrm{i}k_l}\frac{\mathrm{d}\Psi(z_l)}{\mathrm{d}z}\right], \tag{A.7}$$

which enables $\Psi(z_{l-1})$ and $\frac{\mathrm{d}\Psi(z_{l-1})}{\mathrm{d}z}$ to be calculated through equations (A.4) and (A.5).

To implement the algorithm, one can define a vector $\mathbf{X}_l$ whose first component X_l^1 contains the numerical value of $\Psi(z_l)$ and whose second component X_l^2 contains the derivative $\frac{\mathrm{d}\Psi(z_l)}{\mathrm{d}z}$. The full procedure consists then in defining $X_N^1 = \mathrm{e}^{\mathrm{i}k_{\text{III}}D}$ and $X_N^2 = \mathrm{i}k_{\text{III}}\mathrm{e}^{\mathrm{i}k_{\text{III}}D}$. The propagation from $z = D$ to 0 is achieved by applying for $l = N, \ldots, 1$ the relation

$$\begin{pmatrix} X_{l-1}^1 \\ X_{l-1}^2 \end{pmatrix} = \begin{pmatrix} \cos(k_l\Delta z) & -\sin(k_l\Delta z)/k_l \\ k_l \sin(k_l\Delta z) & \cos(k_l\Delta z) \end{pmatrix} \begin{pmatrix} X_l^1 \\ X_l^2 \end{pmatrix}, \tag{A.8}$$

when $E > V_l$ ($k_l = \sqrt{\frac{2m}{\hbar^2}(E - V_l)}$), the relation

$$\begin{pmatrix} X^1_{l-1} \\ X^2_{l-1} \end{pmatrix} = \begin{pmatrix} \cosh(K_l \Delta z) & -\sinh(K_l \Delta z)/K_l \\ -K_l \sinh(K_l \Delta z) & \cosh(K_l \Delta z) \end{pmatrix} \times \begin{pmatrix} X^1_l \\ X^2_l \end{pmatrix}, \tag{A.9}$$

when $E < V_l$ ($K_l = \sqrt{\frac{2m}{\hbar^2}(V_l - E)}$), or the relation

$$\begin{pmatrix} X^1_{l-1} \\ X^2_{l-1} \end{pmatrix} = \begin{pmatrix} 1 & -\Delta z \\ 0 & 1 \end{pmatrix} \begin{pmatrix} X^1_l \\ X^2_l \end{pmatrix}, \tag{A.10}$$

when $E = V_l$. We have finally that

$$A_{\mathrm{I}} = \frac{1}{2}\left[X^1_0 + \frac{1}{\mathrm{i}k_{\mathrm{I}}} X^2_0\right], \tag{A.11}$$

$$B_{\mathrm{I}} = \frac{1}{2}\left[X^1_0 - \frac{1}{\mathrm{i}k_{\mathrm{I}}} X^2_0\right], \tag{A.12}$$

which enables S^{++} and S^{-+} to be calculated from $S^{++} = 1/A_{\mathrm{I}}$ and $S^{-+} = B_{\mathrm{I}}/A_{\mathrm{I}}$.

The 'transmission coefficient' of the potential barrier $V(z)$ at the energy E is finally given by

$$T = \frac{k_{\mathrm{III}}}{k_{\mathrm{I}}} |S^{++}|^2. \tag{A.13}$$

This transmission coefficient T relates the current density J_{in}, which is associated with the incident state Ψ^+_{I} in Region I, to the current density $J_{\mathrm{out}} = T J_{\mathrm{in}}$, which is associated with the transmitted state $S^{++}\Psi^+_{\mathrm{III}}$ in Region III.

This procedure provides the *exact* quantum-mechanical result for the electronic transmission through a barrier that varies in steps in the region $0 \leqslant z \leqslant D$. The accuracy of this approximation can be controlled by letting $\Delta z \to 0$. For three-dimensional problems, it is necessary to apply the layer-addition algorithm presented by Pendry [30] in order to prevent the occurrence of numerical instabilities. This is explained in detail in [31]. The adaptation of the techniques presented in this appendix to the three-dimensional case can be found in [25–28].

References

[1] Xu N S and Huq S E 2005 *Mater. Sci. Eng.* R **48** 47
[2] Fowler R H and Nordheim L W 1928 *Proc. R. Soc.* A **119** 173
[3] Murphy E L and Good R H 1956 *Phys. Rev.* **102** 1464
[4] Good R H and Müller E W 1956 *Handbuch der Physik* vol 21 ed S Flugge (Berlin: Springer) p 176
[5] Young R D 1959 *Phys. Rev.* **113** 110
[6] Stratton R 1964 *Phys. Rev.* **135** A764
[7] Nagy D and Cutler P H 1969 *Phys. Rev.* **186** 651
[8] Swanson L W and Crouser L C 1967 *Phys. Rev.* **163** 622
[9] Gadzuk J W and Plummer E W 1973 *Rev. Mod. Phys.* **45** 487
[10] Miskovsky N M, Park S H, He J and Cutler P H 1993 *J. Vac. Sci. Technol.* B **11** 366
[11] Modinos A 2001 *Solid State Electron.* **45** 809
[12] Forbes R G and Deane J H B 2007 *Proc. R. Soc.* A **463** 2907
[13] Forbes R G 2008 *J. Vac. Sci. Technol.* B **26** 788
[14] Cutler P H, He J, Miskovsky N M, Sullivan T E and Weiss B 1992 *J. Vac. Sci. Technol.* B **11** 387
[15] Jeffreys H 1925 *Proc. Lond. Math. Soc.* **s2–23** 428
[16] Wentzel G 1926 *Z. Phys.* **38** 518
[17] Kramers H A 1926 *Z. Phys.* **33** 828
[18] Brillouin L 1926 *Compt. Rend.* **183** 24
[19] Kemble E C 1935 *Phys. Rev.* **48** 549
[20] Forbes R G 2008 *J. Appl. Phys.* **103** 114911
[21] Landau L D and Lifschitz E M 1958 *Quantum Mechanics* (Oxford: Pergamon)
[22] Vigneron J-P and Lambin P 1980 *J. Phys. A: Math. Gen.* **13** 1135
[23] Nguyen H Q, Cutler P H, Feuchtwang T E, Miskovsky N M and Lucas A A 1985 *Surf. Sci.* **160** 331
[24] Mayer A and Vigneron J-P 1999 *Ultramicroscopy* **79** 35
[25] Mayer A and Vigneron J-P 1997 *Phys. Rev.* B **56** 12599
[26] Mayer A and Vigneron J-P 1999 *Phys. Rev.* B **60** 2875
[27] Mayer A and Vigneron J-P 1999 *J. Vac. Sci. Technol.* B **17** 506
[28] Mayer A, Chung M S, Weiss B L, Miskovsky N M and Cutler P H 2008 *Phys. Rev.* B **78** 205404
[29] Fröman H and Fröman P O 1965 *JWKB Approximation: Contributions to the Theory* (Amsterdam: North-Holland)
[30] Pendry J B 1994 *J. Mod. Opt.* **41** 209
[31] Mayer A and Vigneron J-P 1999 *Phys. Rev.* E **59** 4659