The formal derivation of an exact series expansion for the principal Schottky-Nordheim barrier function $v$, using the Gauss hypergeometric differential equation

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 2008 J. Phys. A: Math. Theor. 41395301
(http://iopscience.iop.org/1751-8121/41/39/395301)
View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.150
The article was downloaded on 03/06/2010 at 07:12

Please note that terms and conditions apply.

# The formal derivation of an exact series expansion for the principal Schottky-Nordheim barrier function $v$, using the Gauss hypergeometric differential equation 

Jonathan H B Deane ${ }^{1}$ and Richard G Forbes ${ }^{2}$<br>${ }^{1}$ Department of Mathematics, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford GU2 7XH, UK<br>${ }^{2}$ Advanced Technology Institute (X1), Faculty of Engineering and Physical Sciences, University of Surrey, Guildford GU2 7XH, UK<br>E-mail: J.Deane@surrey.ac.uk and r.forbes@ieee.org

Received 23 April 2008, in final form 30 July 2008
Published 29 August 2008
Online at stacks.iop.org/JPhysA/41/395301


#### Abstract

The standard theory of Fowler-Nordheim tunnelling and cold field electron emission (CFE) employs a mathematical function $v$, sometimes called the principal field emission elliptic function, but better called the principal Schottky-Nordheim barrier function. This function arises when the simpleJWKB (Jeffreys-Wentzel-Kramers-Brillouin) method is applied to solve the Schrödinger equation approximately, for the image-rounded tunnelling barrier introduced by Schottky and then used by Nordheim in late 1928. An exact series expansion was recently found for $v$, as a function of a complementary elliptic variable $l^{\prime}$ equal to $y^{2}$, where $y$ is the Nordheim parameter. The expansion was originally found by using an algebraic manipulation package. It was subsequently discovered that $v\left(l^{\prime}\right)$ is a particular solution of the ordinary differential equation (ODE) $l^{\prime}\left(1-l^{\prime}\right) \mathrm{d}^{2} v / \mathrm{d} l^{\prime 2}=(3 / 16) v$. This ODE is now recognized to be a special case of the Gauss hypergeometric differential equation. This paper uses known special-case solutions of the hypergeometric equation to formally derive the series expansion for $v\left(l^{\prime}\right)$. It notes how to derive the defining ODE, and then uses an 1876 result from Cayley to derive the boundary condition that $\mathrm{d} v / \mathrm{d} l^{\prime}$ satisfies as $l^{\prime}$ tends to zero. It then establishes the series expansion for $v\left(l^{\prime}\right)$, by applying this and the boundary condition $v(0)=1$. This mathematical derivation underpins earlier results, including good approximate expressions for $v\left(l^{\prime}\right)$. Its outcome proves that terms involving $\ln l^{\prime}$ are part of a mathematically correct solution, but fractional powers of $l^{\prime}$ are not. It also implies that simple Taylor-expansion methods cannot easily generate good approximation formulae valid over the whole range $0 \leqslant l^{\prime} \leqslant 1$; this may also apply to barriers of other shapes. This derivation should bring closure to the particular line of mathematical analysis of CFE theory initiated


by Nordheim in 1928. It is hoped that the derivation might also serve as a model for analysing other tunnelling-barrier problems.

PACS numbers: 79.70.+q, 02.60.Lj

## 1. Introduction

### 1.1. General background

Fowler-Nordheim (FN) tunnelling [1] is electric-field-induced electron tunnelling from a solid or liquid emitter through a roughly triangular barrier. When the emission barrier is strong and the penetration coefficient is small, there is a low-temperature emission regime (including room temperature) known as cold field electron emission (CFE). Tunnelling and CFE are processes of significant technological interest, in particular for the prevention of vacuum breakdown, the development of cold-cathode electron sources and internal electron transfer processes in some electronic devices.

In particular, most forms of high-resolution electron microscope use some type of field emission source, because these have small optical size and are optically very bright. These sources are crucial to many aspects of nanotechnology, because high-resolution electron microscopes are one of the tools that enable us to 'see' at the nanoscale. We believe it appropriate that the mathematics underlying the physics of FN tunnelling should be set out to a standard comparable with that deployed in other basic quantum-mechanical contexts. This paper is part of a process of putting in place what we regard as some necessary links and proofs.

It would have been better if the proof presented here could have been achieved 80 years ago, when the mathematical problem addressed here was first formulated [2], or more than 50 years ago, when a correct numerical solution was first found, by integration using early computers [3]. However, the analytical proof reported here has not previously been available.

The original FN treatment [1] used an exact triangular barrier. This barrier shape is physically unrealistic. Thus, many later treatments modelled tunnelling as taking place through the image-rounded mathematical barrier introduced by Schottky [4] and used by Nordheim [2], called here the 'Schottky-Nordheim (SN) barrier'. For the SN barrier, the variation in electron energy $M$ with distance $z$ is (by definition) given by

$$
\begin{equation*}
M(z)=h-e F z-e^{2} / 16 \pi \epsilon_{0} z \tag{1}
\end{equation*}
$$

where $e$ is the elementary positive charge, $F$ is an electric field that defines the barrier, $h$ is the barrier height when $F=0$ and $\epsilon_{0}$ is the electric constant. $F$ is independent of $z$ and, by convention, is taken as a positive quantity.

For a barrier of this shape, it is mathematically impossible to solve the one-dimensional Schrödinger equation exactly in any simple closed form (see [5]). Thus, normal practice has been to use the so-called simple-JWKB (Jeffreys-Wentzel-Kramers-Brillouin) approximation, developed initially by Jeffreys [6], to derive the following (approximate) expression for the tunnelling probability $D$ :

$$
\begin{equation*}
D \approx \exp \left[-v^{*} b h^{3 / 2} / F\right] \tag{2}
\end{equation*}
$$

Here, $b\left[\equiv(8 \pi / 3)(2 m)^{1 / 2} / e h_{\mathrm{P}}\right]$ is the second FN constant as usually defined (e.g., in [7]), where $m$ is the electron mass in free space and $h_{\mathrm{P}}$ is Planck's constant. $v$ is a mathematical function, well known in field emission, that acts (in the tunnelling exponent) as the barriershape correction factor [7] for this barrier. Although $v$ is sometimes called the 'principal field emission elliptic function', a better name is the 'principal Schottky-Nordheim barrier function'
[7], because $v$ applies specifically to the SN barrier. In equation (2), $v^{*}$ is the particular value of $v$ that corresponds to a barrier defined by particular values of the parameters $h$ and $F$.

Historically [3], $v$ has been expressed as a function of a single mathematical parameter $y$ introduced by Nordheim [2], and a formula has been available to obtain the value of $y$ from the values of $h$ and $F$. Recently [7], however, it has been argued strongly that the natural mathematical variable to use as the argument of $v$ is the so-called complementary elliptic variable $l^{\prime}$. This is equal to $y^{2}$ and is defined by

$$
\begin{equation*}
l^{\prime} \equiv[(1-m) /(1+m)]^{2} \tag{3}
\end{equation*}
$$

where $m$ is the 'elliptic parameter' used in modern elliptic-function theory and defined in [8] (also see (9)). The primed symbol $l^{\prime}$ was chosen, following a normal convention in elliptic-function theory, because $l^{\prime}$ is a 'complementary' variable in the sense that $l^{\prime} \rightarrow 0$ as $m \rightarrow 1$.

Integration of (2) over all travelling electron states occupied in the emitter at 0 K leads, for a free-electron model of the emitter, to the so-called standard FN-type equation for the emission current density $J$ :

$$
\begin{equation*}
J=t_{\mathrm{F}}^{-2} a \phi^{-1} F^{2} \exp \left[-v_{\mathrm{F}} b \phi^{3 / 2} / F\right] \tag{4}
\end{equation*}
$$

where $\phi$ is the local work-function and $a\left[\equiv e^{3} / 8 \pi h_{\mathrm{P}}\right]$ is the first FN constant as usually defined [7]. Here, $t$ is a mathematical function defined [7] by

$$
\begin{equation*}
t\left(l^{\prime}\right)=v\left(l^{\prime}\right)-(4 / 3) l^{\prime} \mathrm{d} v / \mathrm{d} l^{\prime} \tag{5}
\end{equation*}
$$

and $v_{\mathrm{F}}$ and $t_{\mathrm{F}}$ are values of $v$ and $t$ that apply to a barrier for which the zero-field height (i.e., height for zero applied field $F$ ) is $\phi$. Equation (4) was developed by Murphy and Good [9] from earlier work; its derivation has been reworked by Forbes and Deane [7], using $l^{\prime}$ rather than $y$. When $v_{\mathrm{F}}$ and $t_{\mathrm{F}}$ are evaluated, $l^{\prime}$ is set equal to the physical 'scaled barrier field' $f$ defined by $f=F / F_{\phi}$, where $F_{\phi}$ is the barrier field necessary to reduce to zero a tunnelling barrier initially of height $\phi$. Approximations for the function $v$ and related functions have played a large role in the analysis of experimental CFE data for the last 50 years.

### 1.2. Mathematical context

Historically, definitions of $v$ have been framed either in terms of an integral derived from the simple-JWKB treatment of the tunnelling barrier [7, 9], or in terms of a derived expression $[9,10]$ (see (10)) involving the complete elliptic integrals [8] $K$ and $E$. But recently an explicit series expansion (42) was discovered $[7,11]$ for $v\left(l^{\prime}\right)$, by using the computer algebra package MAPLE to expand the definition involving $K$ and $E$.

Numerical estimates of $v\left(l^{\prime}\right)$ made using MAPLE agreed with values obtained by numerical evaluation of the relevant JWKB integral, to better than 12 decimal places, showing both methods to be mathematically sound. We subsequently found algebraic formulae that reproduced the MAPLE result (see [7], appendix A). However, manual derivation of higher order terms in the series was excessively laborious; also, this method does not bring out the underlying mathematics.

Knowing the form of the exact expansion for $v\left(l^{\prime}\right)$ enabled us to develop new approximation formulae for $v\left(l^{\prime}\right)$ and $\mathrm{d} v / \mathrm{d} l^{\prime}$. These have absolute error $|\epsilon|<8 \times 10^{-10}$, and substantially outperform earlier numerical approximations of equivalent complexity [12]. The form of the exact expansion also explains the mathematical success of the simple approximation formula $[7,11]$

$$
\begin{equation*}
v\left(l^{\prime}\right) \approx 1-l^{\prime}+(1 / 6) l^{\prime} \ln l^{\prime} \tag{6}
\end{equation*}
$$

This formula has the merits that it is exact at $l^{\prime}=0$ and $l^{\prime}=1$, and (when assessed over the whole range $0 \leqslant l^{\prime} \leqslant 1$ ) has absolute error $|\epsilon|<0.0025$, thereby outperforming all existing formulae of equivalent complexity. Formula (6) seems likely to have a considerable impact in CFE theory [7, 13, 14]. We have been interested in the mathematical origin of these successes.

In seeking deeper understanding, we established [7] that $v\left(l^{\prime}\right)$ is a particular solution of the ordinary differential equation (ODE):

$$
\begin{equation*}
l^{\prime}\left(1-l^{\prime}\right) \frac{\mathrm{d}^{2} W}{\mathrm{~d} l^{\prime 2}}=\frac{3}{16} W \tag{7}
\end{equation*}
$$

subject to the boundary condition $v(0)=1$ and a second boundary condition derived below.
It is possible to treat (7) as an equation of mathematical physics in own right and to derive two independent solutions from first principles, using the method of Frobenius. We have confirmed [15] that this leads correctly to (42). However, we have now recognized ${ }^{1}$ that (7) is a special case of the Gauss hypergeometric differential equation

$$
\begin{equation*}
l^{\prime}\left(1-l^{\prime}\right) \frac{\mathrm{d}^{2} W}{\mathrm{~d} l^{\prime 2}}+\left[\gamma-(\alpha+\beta+1) l^{\prime}\right] \frac{\mathrm{d} W}{\mathrm{~d} l^{\prime}}-\alpha \beta W=0 \tag{8}
\end{equation*}
$$

in which the Gauss coefficients take the values $\alpha=-3 / 4, \beta=-1 / 4, \gamma=0$. Independent solutions for this special case are known (e.g., [8]), so it is more appropriate to start from these.

This paper aims to record, for archival purposes, the formal mathematical derivation of expansion (42). Section 2 recapitulates the derivation of (7). Section 3 establishes the boundary conditions that $v\left(l^{\prime}\right)$ must satisfy. Section 4 uses a well-defined form [8] for the independent solutions of (7) to establish the series expansion for $v\left(l^{\prime}\right)$. Section 5 provides discussion.

## 2. Derivation of defining equation

The derivation of (7) was outlined in [7]; for completeness here, we give the proof in slightly more detail. The complete elliptic integrals of the first $(K)$ and second $(E)$ kinds can be defined in terms of the elliptic parameter $m$ by [8]

$$
\begin{equation*}
K(m)=\int_{0}^{\pi / 2} \frac{\mathrm{~d} \phi}{\sqrt{1-m \sin ^{2} \phi}} \quad \text { and } \quad E(m)=\int_{0}^{\pi / 2} \sqrt{1-m \sin ^{2} \phi} \mathrm{~d} \phi \tag{9}
\end{equation*}
$$

Equation (26a) in [10] gives a formula for $v(y)$, originally derived by Murphy and Good [9]:

$$
\begin{equation*}
v(y)=(1+y)^{1 / 2}[E(m(y))-y K(m(y))], \tag{10}
\end{equation*}
$$

where $m$ here is the parameter denoted by $m^{*}$ in [10]. Comparison of definition (3) here with definition (26b) in [10] confirms that $y \equiv \sqrt{l^{\prime}}$, so-expressed in terms of $l^{\prime}$-equation (10) becomes

$$
\begin{equation*}
v\left(l^{\prime}\right)=\left(1+\sqrt{l^{\prime}}\right)^{1 / 2}\left[E\left(m\left(l^{\prime}\right)\right)-\sqrt{l^{\prime}} K\left(m\left(l^{\prime}\right)\right)\right] . \tag{11}
\end{equation*}
$$

Equation (29) in [10] provides the further result:

$$
\begin{equation*}
\mathrm{d} v / \mathrm{d} y=-(3 / 2) y(1+y)^{-1 / 2} K(m(y)) \tag{12}
\end{equation*}
$$

Noting that $\mathrm{d} y / \mathrm{d} l^{\prime}=1 /\left(2 \sqrt{l^{\prime}}\right)$, we obtain

$$
\begin{equation*}
\mathrm{d} v / \mathrm{d} l^{\prime}=-(3 / 4)\left(1+\sqrt{l^{\prime}}\right)^{-1 / 2} K\left(m\left(l^{\prime}\right)\right) \tag{13}
\end{equation*}
$$

A further differentiation with respect to $l^{\prime}$ then gives

$$
\begin{equation*}
\mathrm{d}^{2} v / \mathrm{d} l^{\prime 2}=-(3 / 16)\left(1+\sqrt{l^{\prime}}\right)^{-1 / 2}\left[4 \frac{\mathrm{~d} K}{\mathrm{~d} l^{\prime}}-\frac{K}{\sqrt{l^{\prime}}\left(1+\sqrt{l^{\prime}}\right)}\right] \tag{14}
\end{equation*}
$$

From equation (27) in [10], we have

$$
\begin{equation*}
\mathrm{d} K / \mathrm{d} m=[E-(1-m) K] / 2 m(1-m) \tag{15}
\end{equation*}
$$

[^0]From (3)

$$
\begin{align*}
& m\left(l^{\prime}\right)=\left(1-\sqrt{l^{\prime}}\right) /\left(1+\sqrt{l^{\prime}}\right),  \tag{16}\\
& \mathrm{d} m / \mathrm{d} l^{\prime}=-1 /\left[\left(\sqrt{l^{\prime}}\right)\left(1+\sqrt{l^{\prime}}\right)^{2}\right] \tag{17}
\end{align*}
$$

Using (16) and then (17) to put $\mathrm{d} K / \mathrm{d} m$ in terms of $l^{\prime}$, we obtain

$$
\begin{align*}
\mathrm{d} K / \mathrm{d} m & =\frac{\left(1+\sqrt{l^{\prime}}\right) E-2 \sqrt{l^{\prime}}\left(1+\sqrt{l^{\prime}}\right) K}{4 \sqrt{l^{\prime}}\left(1-\sqrt{l^{\prime}}\right)}  \tag{18}\\
\mathrm{d} K / \mathrm{d} l^{\prime} & =-\frac{\left(1+\sqrt{l^{\prime}}\right) E-2 \sqrt{l^{\prime}} K}{4 l^{\prime}\left(1-l^{\prime}\right)} \tag{19}
\end{align*}
$$

Substitution of (19) into (14) then yields
$l^{\prime}\left(1-l^{\prime}\right) \mathrm{d}^{2} v / \mathrm{d} l^{\prime 2}=(3 / 16)\left(1+\sqrt{l^{\prime}}\right)^{-1 / 2}\left[\left(1+\sqrt{l^{\prime}}\right) E-2\left(\sqrt{l^{\prime}}\right) K+\sqrt{l^{\prime}}\left(1-\sqrt{l^{\prime}}\right) K\right]$,
$l^{\prime}\left(1-l^{\prime}\right) \mathrm{d}^{2} v / \mathrm{d} l^{\prime 2}=(3 / 16) v$.
This shows that $v$ is a particular solution of ODE (7).

## 3. Boundary conditions

We require the boundary conditions that $v\left(l^{\prime}\right)$ and $\mathrm{d} v / \mathrm{d} l^{\prime}$ satisfy at $l^{\prime}=0$. It is well known in CFE theory that $v(0)=1$. However, $\mathrm{d} v / \mathrm{d} l^{\prime}$ becomes infinite as $l^{\prime} \rightarrow 0$, so the boundary condition on $\mathrm{d} v / \mathrm{d} l^{\prime}$ has to take the slightly unusual form that ' $\mathrm{d} v / \mathrm{d} l^{\prime}$ becomes infinite in the correct way'. We develop both conditions formally from a result originally proved by Cayley [17] in 1876, via three lemmas.

Lemma 1. As $l^{\prime}$ approaches zero from above, the function $K\left(m\left(l^{\prime}\right)\right)$ is given by

$$
\begin{equation*}
K\left(m\left(l^{\prime}\right)\right)=(3 / 2) \ln 2-(1 / 4) \ln l^{\prime}+O\left(\sqrt{l^{\prime}}\right) \tag{21}
\end{equation*}
$$

Proof. From (16), we have

$$
(1-m)=\frac{2 \sqrt{l^{\prime}}}{1+\sqrt{l^{\prime}}}
$$

Formula 17.3.26 in [8] is derived from Cayley's result and states that

$$
\lim _{m \rightarrow 1} K(m)=\ln [4 / \sqrt{(1-m)}]
$$

Hence
$\lim _{l^{\prime} \rightarrow 0} K\left(m\left(l^{\prime}\right)\right)=\lim _{l^{\prime} \rightarrow 0} \ln \left[4 \sqrt{\frac{1+\sqrt{l^{\prime}}}{2 \sqrt{l^{\prime}}}}\right]=\lim _{l^{\prime} \rightarrow 0}\left[(3 / 2) \ln 2-(1 / 4) \ln l^{\prime}+O\left(\sqrt{l^{\prime}}\right)\right]$,
as required.
We have thus proved a Cayley-type result for $K$ as a function of $l^{\prime}$. This result is key to deriving the series expansion for $v$.

Lemma 2. $v(0)=1$.
Proof. Using lemma 1, we find that, in the limit of small $l^{\prime}$, the term involving $K\left(m\left(l^{\prime}\right)\right)$ in definition (11) takes the form

$$
-\lim _{l^{\prime} \rightarrow 0}\left[\left(1+\sqrt{l^{\prime}}\right)^{1 / 2} \sqrt{l^{\prime}}\left[(3 / 2) \ln 2-(1 / 4) \ln l^{\prime}\right]\right]=0
$$

When $l^{\prime}=0$, then $m=1$, and the term in $E\left(m\left(l^{\prime}\right)\right)$ in (11) reduces to

$$
E(m=1)=\int_{0}^{\pi / 2} \cos \phi \mathrm{~d} \phi=1 .
$$

It follows that $v(0)=1$. This is a well-known result in CFE theory, but for completeness we have given formal proof here.

## Lemma 3.

$$
\begin{equation*}
\lim _{l^{\prime} \rightarrow 0}\left\{\mathrm{~d} v / \mathrm{d} l^{\prime}-(3 / 16) \ln l^{\prime}\right\}=-(9 / 8) \ln 2 \tag{22}
\end{equation*}
$$

Proof. From (13) and (21) we have, in the limit of small $l^{\prime}$, that

$$
\frac{\mathrm{d} v}{\mathrm{~d} l^{\prime}} \approx-\frac{3}{4}\left(1-\frac{\sqrt{l^{\prime}}}{2}\right)\left(\frac{3}{2} \ln 2-\frac{1}{4} \ln l^{\prime}\right)
$$

The limiting form for $\mathrm{d} v / \mathrm{d} l^{\prime}$ in (22) follows.

## 4. Derivation of the series expansion for $\boldsymbol{v}\left(\boldsymbol{l}^{\prime}\right)$

Obviously, (7) has two independent solutions. A complication is that different reference sources on the hypergeometric equation give different forms for the second solution. There are numerous legitimate forms, but one or two of the standard reference sources seem to contain errors or misprints. In this paper we start from formulae 15.5.20 and 15.5.21 in [8]; these do yield what we know, from our earlier work, to be the correct result. These independent solutions of (7) are denoted here by $W_{\mathrm{A}}\left(l^{\prime}\right)$ and $W_{\mathrm{M}}\left(l^{\prime}\right)$.

### 4.1. The Gauss hypergeometric series

The Gauss hypergeometric function $F\left(p, q ; r ; l^{\prime}\right)$ can be written as the series expansion
$F\left(p, q ; r ; l^{\prime}\right)=1+\frac{p q}{1!r} l^{\prime}+\frac{p(p+1) q(q+1)}{2!r(r+1)} l^{\prime 2}+\cdots \equiv \sum_{i=0}^{\infty} \frac{(p)_{i}(q)_{i}}{i!(r)_{i}} l^{\prime i} \equiv \sum_{i=0}^{\infty} a_{i} l^{\prime i}$,
where the Pochhammer symbol (or 'rising factorial') $(p)_{i}$ is defined by

$$
\begin{equation*}
(p)_{0}=1, \quad(p)_{i}=p(p+1) \cdots(p+i-1), \quad(i \geqslant 1) \tag{24}
\end{equation*}
$$

There also exists a recurrence relation for the coefficients $a_{i}$ :

$$
\begin{equation*}
a_{0}=1, \quad a_{i+1}=\frac{(p+i)(q+i)}{(i+1)(r+i)} a_{i}, \quad(i \geqslant 0) . \tag{25}
\end{equation*}
$$

For the values $\alpha=-3 / 4, \beta=-1 / 4, \gamma=0$ specified earlier, the parameters used in chapter 15 of [8] have the values $a=-3 / 4, b=-1 / 4, m=1, z=l^{\prime}$. So, from formulae there, the arguments of our function $F\left(p, q ; r ; l^{\prime}\right)$ have the values $p=1 / 4, q=3 / 4, r=2$. The summation index $n$ in [8] will be replaced by $i$ here, to avoid a clash with notation we have used elsewhere [7].

### 4.2. First independent solution

Formula 15.5 .20 in [8] thus yields

$$
\begin{gather*}
W_{\mathrm{A}}\left(l^{\prime}\right)=l^{\prime} F\left(\frac{1}{4}, \frac{3}{4} ; 2 ; l^{\prime}\right)=l^{\prime} \sum_{i=0}^{\infty} a_{i} l^{l^{i}},  \tag{26}\\
a_{0}=1, \quad a_{i+1}=\frac{(1 / 4+i)(3 / 4+i)}{(i+1)(2+i)} a_{i}=\frac{i(i+1)+(3 / 16)}{(i+1)(i+2)} a_{i}=\frac{16 i(i+1)+3}{16(i+1)(i+2)} a_{i} . \tag{27}
\end{gather*}
$$

Alternatively, an explicit expression for $a_{i}(i \geqslant 1)$ can be obtained as follows. From the definition of the Pochhammer symbol, we find that $(2)_{i}=(i+1)$ ! and

$$
\begin{aligned}
\left(\frac{1}{4}\right)_{i}\left(\frac{3}{4}\right)_{i} & =\overbrace{\left[\frac{1}{4} \cdot \frac{5}{4} \cdot \frac{9}{4} \cdots \frac{4 i-3}{4}\right]}^{i \text { terms }} \cdot \overbrace{\left[\frac{3}{4} \cdot \frac{7}{4} \cdot \frac{11}{4} \cdots \frac{4 i-1}{4}\right]}^{i \text { terms }} \\
& =\frac{1 \cdot 3 \cdot 5 \cdots(4 i-1)}{2^{4 i}}=\frac{(4 i-1)!}{2^{4 i}(2 i-1)!2^{2 i-1}} .
\end{aligned}
$$

Hence, we find

$$
\begin{equation*}
a_{i}=\frac{(4 i-1)!}{2^{6 i-1} i!(i+1)!(2 i-1)!}, \quad(i \geqslant 1) \tag{28}
\end{equation*}
$$

The first three values of $a_{i}$ are $a_{0}=1, a_{1}=3 / 32, a_{2}=35 / 1024$, so the lowest terms of the series for $W_{\mathrm{A}}\left(l^{\prime}\right)$ are

$$
\begin{equation*}
W_{\mathrm{A}}\left(l^{\prime}\right)=l^{\prime}\left[1+\frac{3}{32} l^{\prime}+\frac{35}{1024} l^{\prime 2}+O\left(l^{\prime 3}\right)\right] . \tag{29}
\end{equation*}
$$

### 4.3. Second independent solution

Formula 15.5 .21 in [8] yields
$W_{\mathrm{M}}\left(l^{\prime}\right)=l^{\prime} \ln l^{\prime} F\left(\frac{1}{4}, \frac{3}{4} ; 2 ; l^{\prime}\right)+l^{\prime} \sum_{i=1}^{\infty} l^{\prime i} \frac{(1 / 4)_{i}(3 / 4)_{i}}{(2)_{i} i!} k_{i}-\sum_{i=1}^{1} l^{l^{i}} \frac{(i-1)!(-1)_{i}}{(3 / 4)_{i}(1 / 4)_{i}} l^{\prime 1-i}$,
where $k_{i}$ is given in terms of the $\psi$-function $[8,16]$ by
$k_{i}=\psi(i+1 / 4)-\psi(1 / 4)+\psi(i+3 / 4)-\psi(3 / 4)-\psi(i+2)+\psi(2)-\psi(i+1)+\psi(1)$,
$\psi(x)=\frac{\mathrm{d}}{\mathrm{d} x} \ln \Gamma(x)$,
$\Gamma(x)=\int_{0}^{\infty} t^{x-1} \mathrm{e}^{-t} \mathrm{~d} t$.
The form of (30) is easily simplified. (i) The hypergeometric function can be replaced by its series expansion in terms of the coefficients $a_{i}$, as above. (ii) The Pochhammer terms in the first summation are part of the definition of $a_{i}$. Further, (31) allows us to define $k_{0}=0$, and make the lower limit in this summation $i=0$. (iii) The second summation consists of a single term, which has the value $-16 / 3$. So (30) becomes

$$
\begin{equation*}
W_{\mathrm{M}}\left(l^{\prime}\right)=16 / 3+l^{\prime} \ln l^{\prime} \sum_{i=0}^{\infty} a_{i} l^{\prime i}+l^{\prime} \sum_{i=0}^{\infty} a_{i} k_{i} l^{\prime i} \tag{34}
\end{equation*}
$$

Using the property $[8,16]$ that $\psi(x+1)=\psi(x)+1 / x$, which is valid for all positive values of $x$ and for negative non-integral values of $x$ [16], we have

$$
\begin{equation*}
k_{i+1}=k_{i}+(i+1 / 4)^{-1}+(i+3 / 4)^{-1}-(i+1)^{-1}-(i+2)^{-1} . \tag{35}
\end{equation*}
$$

So we obtain the recurrence formula (for $i \geqslant 0$ )

$$
\begin{equation*}
k_{0}=0, \quad k_{i+1}=k_{i}+\frac{32 i^{2}+58 i+23}{(4 i+1)(4 i+3)(i+1)(i+2)} \tag{36}
\end{equation*}
$$

The first three values of $k_{i}$ are $0,23 / 6,153 / 35$, so the lowest terms in the series expansion for $W_{\mathrm{M}}\left(l^{\prime}\right)$ are
$W_{\mathrm{M}}\left(l^{\prime}\right)=\frac{16}{3}+l^{\prime}\left[\frac{23}{64} l^{\prime}+\frac{153}{1024} l^{\prime 2}+O\left(l^{\prime 3}\right)\right]+l^{\prime} \ln l^{\prime}\left[1+\frac{3}{32} l^{\prime}+\frac{35}{1024} l^{\prime 2}+O\left(l^{\prime 3}\right)\right]$.

### 4.4. Derivation of $v\left(l^{\prime}\right)$ as a particular solution

The particular solution $v\left(l^{\prime}\right)$ takes the form $v\left(l^{\prime}\right)=A_{\mathrm{M}} W_{\mathrm{A}}+C_{\mathrm{M}} W_{\mathrm{M}}$, where $A_{\mathrm{M}}$ and $C_{\mathrm{M}}$ are constants to be determined. (These constants are different from those we have used elsewhere, because we are now using the form in [8] for the second independent solution.) In terms of these constants, the lowest terms of the expansions for $v\left(l^{\prime}\right)$ and $\mathrm{d} v / \mathrm{d} l^{\prime}$ are

$$
\begin{align*}
& v\left(l^{\prime}\right)=A_{\mathrm{M}} l^{\prime}+C_{\mathrm{M}}\left[16 / 3+l^{\prime} \ln l^{\prime}\right]+O\left(l^{\prime 2}\right),  \tag{38}\\
& \mathrm{d} v / \mathrm{d} l^{\prime}=A_{\mathrm{M}}+C_{\mathrm{M}}\left[1+\ln l^{\prime}\right]+O\left(l^{\prime}\right) . \tag{39}
\end{align*}
$$

The boundary condition $v(0)=1$ yields $C_{\mathrm{M}}=3 / 16$. Condition (22) then yields

$$
\begin{equation*}
-\frac{9}{8} \ln 2=\lim _{l^{\prime} \rightarrow 0}\left\{\frac{\mathrm{~d} v}{\mathrm{~d} l^{\prime}}-\frac{3}{16} \ln l^{\prime}\right\}=A_{\mathrm{M}}+\frac{3}{16} \tag{40}
\end{equation*}
$$

So $A_{\mathrm{M}}=-(9 / 8) \ln 2-3 / 16$, and the series expansion for $v\left(l^{\prime}\right)$ takes the form

$$
\begin{equation*}
v\left(l^{\prime}\right)=1+\sum_{i=0}^{\infty} a_{i} l^{\prime i+1}\left[-\frac{9}{8} \ln 2+\frac{3}{16}\left(k_{i}-1\right)+\frac{3}{16} \ln l^{\prime}\right] \tag{41}
\end{equation*}
$$

The lowest few terms of this series are

$$
\begin{gather*}
v\left(l^{\prime}\right)=1-\left(\frac{9}{8} \ln 2+\frac{3}{16}\right) l^{\prime}-\left(\frac{27}{256} \ln 2-\frac{51}{1024}\right) l^{\prime 2}-\left(\frac{315}{8192} \ln 2-\frac{177}{8192}\right) l^{\prime 3}+O\left(l^{\prime 4}\right) \\
+l^{\prime} \ln l^{\prime}\left[\frac{3}{16}+\frac{9}{512} l^{\prime}+\frac{105}{16384} l^{\prime 2}+O\left(l^{\prime 3}\right)\right] \tag{42}
\end{gather*}
$$

This is the series originally discovered [11] using MAPLE, here written in terms of $l^{\prime}$ rather than $y$. Its further development, to obtain useful approximation formulae, is described in [7].

## 5. Discussion

For most of the last 50 years, the function $v$ has been expressed in CFE theory as a function of the Nordheim parameter $y$. In [11] was argued that, because the discovered series contained no power terms in odd powers of $y$, it would be mathematically more natural to use $l\left\lceil\left[\equiv y^{2}\right]\right.$ as the independent variable. The derivation here confirms that fractional powers of $l^{\prime}$ do not appear in the mathematically correct expansion for $v\left(l^{\prime}\right)$, but that terms in $\ln l^{\prime}$ are an intrinsic part of it. As discussed in [7], using $l^{\prime}$ in the mathematics means that the natural parameter to use in related physical discussions is the scaled barrier field $f$.

Formulae such as (42) and (6) cannot easily be derived by simple Taylor expansion methods, because such methods do not generate terms in $\ln l^{\prime}$. It follows that, for the SN barrier, simple Taylor-expansion methods do not work well: for the exponent correction factor, it is not easy to use them to generate good approximate formulae that are valid for the whole range $0 \leqslant l^{\prime} \leqslant 1$. This conclusion may also be applicable to tunnelling barriers of other shapes.

The algebraic manipulation package MAPLE played a crucial role in stimulating this work, because the MAPLE result [11] drew attention to the existence and form of the series expansion for $v$, thus providing a result to aim for. Derivation of the $v\left(l^{\prime}\right)$ expansion by finding series expansions for $K\left(l^{\prime}\right)$ and $E\left(l^{\prime}\right)$, and then inserting them into (11), proved excessively laborious if performed by hand [7], even after we had found the Cayley forms [17] for the expansions of $K(m)$ and $E(m)$. So we looked for a mathematical alternative.

Much of sections 3 and 4 could, in principle, have been written many years ago, but there was no incentive. The analysis has been made readily achievable, rather than so complex as to be unlikely to happen, by the relatively recent introduction of reliable computer algebra
packages. Perhaps, overall, it is not entirely surprising that getting a well-proven series expansion/definition for $v$ in place has taken nearly 80 years, measured from Nordheim's original [2] (incorrect [3]) attempt to derive an exponent correction factor for the SN barrier.

This derivation will, we think, bring closure to the particular mathematical analysis of CFE, based on the simple-JWKB approximation, that was initiated by Nordheim in late 1928. We hope that our derivation might also be able to serve as a prototype for the treatment of other barrier models, particularly for realistic models for the potential energy variation above sharply curved emitters. The keys, in each case, would be to find an ODE that the tunnellingexponent correction function satisfies, and a suitable formulation of the boundary conditions. It remains to be established whether this is mathematically possible.

## References

[1] Fowler R H and Nordheim L W 1928 Electron emission in intense electric fields Proc. R. Soc. Lond. A 119 173-81
[2] Nordheim L W 1928 The effect of the image force on the emission and reflexion of electrons by metals Proc. R. Soc. Lond. A 121 626-39
[3] Burgess R F, Kroemer H and Houston J M 1953 Corrected values of Fowler-Nordheim field emission functions $v(y)$ and $s(y)$ Phys. Rev. 90515
[4] Schottky W 1914 Über den Einfluss von Strukturwirkungen, besonders der Thomsonschen Bildkraft, auf die Elektronenemission der Metalle Phys. Z. 15 872-8
[5] Fröman H and Fröman P O 1965 JWKB Approximation-Contributions to the Theory (Amsterdam: NorthHolland)
[6] Jeffreys H 1924 On certain approximate solutions of linear differential equations of the second order Proc. Lond. Math. Soc. 23 428-36
[7] Forbes R G and Deane J H B 2007 Reformulation of the Standard Theory of Fowler-Nordheim tunneling and cold field electron emission Proc. R. Soc. Lond. A 463 2907-27
[8] Abramowitz M and Stegun I A (ed) 1965 Handbook of Mathematical Functions (New York: Dover)
[9] Murphy E L and Good R H 1956 Thermionic emission, field emission and the transition regime Phys. Rev. 102 1464-73
[10] Forbes R G 1999 Use of a spreadsheet for Fowler-Nordheim equation calculations J. Vac. Sci. Technol. B 17 534-41
[11] Forbes R G 2006 Simple good approximations for the special elliptic functions in the JWKB theory of FowlerNordheim tunneling through a Schottky-Nordheim barrier Appl. Phys. Lett. 89113122
[12] Hastings C Jr 1955 Approximations for Digital Computers (Princeton, NJ: Princeton University Press)
[13] Jensen K L 2007 Electron Emission Physics (Adv. Imaging Electron Phys. vol 149) (Amsterdam: Elsevier) pp 1-337
[14] Forbes R G 2008 Call for experimental test of a revised mathematical form for empirical field emission current-voltage characteristics Appl. Phys. Lett. 92193105
[15] Deane J H B, Forbes R G and Shail R W 2007 Formal derivation of an exact series expansion for the principal field emission elliptic function $v$ Preprint arXiv:0708.0996
[16] Ross B 1978 The Psi function Math. Mag. 51 (3) 176-9
[17] Cayley A 1876 An Elementary Treatise on Elliptic Functions (Cambridge: Deighton Bell) pp 46-55


[^0]:    1 We thank an anonymous referee, for an earlier submission, for pointing this out.

