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Tunnelling through rough barriers

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Abstract. The mean current density through tunnelling barriers with rough surfaces is considered. Special attention is paid to the current-bias characteristic. The roughness is modelled by uniformly distributed short-ranged bumps. It is found that roughness causes a change of the effective barrier thickness according to the mean height deviation from the ideal surface and gives rise to a diffuse current contribution that enhances the current through the barrier. A generalization of the results using the local density of states is given.

1. Introduction

During the last decade, great progress in thin-film technology has made it possible to produce ultra-thin layers of high quality. For example, AlGaAs layers can be grown that show perfectly abrupt interfaces [1]. Nevertheless, the surface roughness of thin films is a point still under discussion [2–5] because it strongly influences transport properties [6, 7].

Recently, a bimodal roughness spectrum has been proposed [8] and experimentally investigated [4, 9, 10]. Following the ideas in [8], the interface roughness spectrum can be described by a long-wave part due to large islands of constant film thickness and a part due to microroughness on an atomic scale.

The present paper addresses the microroughness of a biased tunnel barrier and its influence on the current passing through the barrier. The current through rough tunnelling barriers has already been the focus of a paper by Houzé and Boyer [11] where large-scale roughness between macroscopic contacts was considered. Other related work has been done by Knauer and co-workers [12] and Stoll and Schneider [13] who considered disordered tunnel barriers, and by Leo and MacDonald [14], Tan and co-workers [15] and Johansson [16], who treated interface roughness in resonant double-barrier structures. The similar problem of photon tunnelling through thin layers with uneven surfaces was the focus of [17] and [18].

In the present paper, surface roughness is modelled by uncorrelatedly distributed bumps that cover the barrier with a main density $\mathcal{N}$ [6]. These can be either concave or convex. Their characteristic dimensions are small compared to the de Broglie wavelength of the tunnelling particles. The calculations are based on a scattering picture that uses the individual scattering amplitude $f^{(n)}$ of each bump. However, since we are interested in the mean current density that passes through the barrier, the final results obtained here contain averaged quantities such as $\langle f\rangle$ and $\langle |f|^2\rangle$. Although our method is quite similar to that of Leo and MacDonald [14], the results obtained here within the consequent scattering picture can be represented very compactly and transparently by taking advantage of the optical theorem in simplifying some expressions. Moreover, the method presented can

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be applied without any changes to small particles adsorbed on the tunnel barrier if their characteristic $\langle f \rangle$ and $\langle |f|^2 \rangle$ are known. In principle, the scattering amplitude of each *individual bump can be obtained exactly. The multiple-scattering effects between them,* however, are neglected here in order to keep the problem treatable.

In contrast to calculations on barriers with constant thickness where a one-dimensional treatment is often sufficient [19], the present investigation, which includes scattering, must be essentially three dimensional. We adopt the Fourier transformation method employed in [12]. This allows a transparent and compact formulation of the results.

The paper is organized as follows. In section 2, an analytical expression for the tunnelling current through the rough barrier is derived. Section 3 illuminates the problem from a more general point of view, giving a reformulation of the results useful for a discrete set of possible scattering states. Conclusions and an outlook are presented in section 4. An appendix shows the treatment of a trapezoidal barrier potential.

2. The tunnelling current

Our model consists of a tunnel barrier of thickness L that is embedded in two regions with zero potential (on the left-hand side, $z < 0$) and with a bias potential (on the right-hand side, $z > L$), respectively (see figure 1). The bias is assumed to be small compared to the barrier height. The z-dependent potential profile is

$$z < 0\colon\ V(z) = 0 \qquad 0 \leqslant z \leqslant L\colon\ V(z) = \frac{\hbar^2 v(z)}{2m} \qquad z > L\colon\ V(z) = W = \frac{\hbar^2 w}{2m}. \tag{1}$$

The barrier surface at $z = 0$ is roughened by uncorrelated bumps with a mean surface density $\mathcal{N}$. Each of them can be vaulted outward as well as inward and is characterized by its individual scattering amplitude $f^{(n)}$. Multiple-scattering effects between them are neglected.

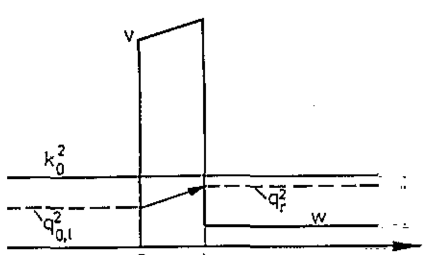

Figure 1. Energy scheme of the barrier model (thick line) and possible scattering event of a particle incident on the barrier with a (normalized) energy k^2. The particle is scattered from the initial state with a normal momentum component $q_{0,l}$ into one with $q_r > q_{0,l}$.

If a primary field $\phi_0(\boldsymbol{r})$ with energy $E = (\hbar^2/2m)k^2$ is incident on the barrier, it will be scattered at the bumps. The resulting total field is the superposition of $\phi_0(\boldsymbol{r})$ and scattered waves

$$\Psi(\boldsymbol{r}) = \phi_0(\boldsymbol{r}) + \sum_n f^{(n)}\phi_0(\boldsymbol{r}_n)G(\boldsymbol{r}, \boldsymbol{r}_n) \qquad \boldsymbol{r} \equiv (\boldsymbol{R}, z) \tag{2}$$

where $\boldsymbol{r}_n = (\boldsymbol{R}_n, 0)$ is the position of the nth bump. $G(\boldsymbol{r}, \boldsymbol{r}')$ is the propagator of the system without roughness. It satisfies the differential equation

$$\left(\Delta + k^2 - \frac{2m}{\hbar^2}V(z)\right) G(\boldsymbol{r}, \boldsymbol{r}') = -\delta(\boldsymbol{r}, \boldsymbol{r}') \tag{3}$$

and can be decomposed into one-dimensional components $G_p(z, z')$ by means of the Fourier transformation

$$G(r, r') = \frac{1}{(2\pi)^2} \int d^2 p\, e^{ip\cdot(R-R')} G_p(z, z') \tag{4}$$

where $G_p(z, z')$ obeys the equation

$$\left(\frac{\partial^2}{\partial z^2} + k^2 - \frac{2m}{\hbar^2} V(z) - p^2\right) G_p(z, z') = -\delta(z, z'). \tag{5}$$

For $z' \leqslant 0$, $z \geqslant L$, $G_p(z, z')$ can be represented as

$$G_p(z, z') = \frac{i e^{-iq_l z'} t(q_l) e^{iq_r z}}{2q_l} \tag{6}$$

with $q_l^2 = k^2 - p^2$ and $q_r^2 = k^2 - p^2 - w$. $t(q_l)$ is the one-dimensional transmission coefficient for a wave $e^{iq_l z}$ originating from $z < 0$. If both arguments lie on the left-hand side, $z, z' \leqslant 0$, $G_p(z, z')$ reads

$$G_p(z, z') = \frac{i}{2q_l} [e^{iq_l|z-z'|} + r(q_l) e^{iq_l|z+z'|}]. \tag{7}$$

$r(q_l)$ is the 1D reflection coefficient of the barrier.

Now we assume a plane wave $\exp[i(p_0 \cdot R + q_{0,l} z)]$ to be incident on the barrier from the left under an angle $\varphi_0 = \cos^{-1}(q_{0,l}/k)$. Our goal is to calculate the current density $\langle j_z \rangle$ that passes through the rough barrier, averaged over all bump configurations. In particular, we are interested in the dependence of $\langle j_z \rangle$ on the bias w. $\langle j_z \rangle$ depends on the bias w only via q_r. We insert (2), (4), (6), (7) into the general formula

$$\langle j_z \rangle = \lim_{A,N\to\infty} \frac{1}{A^N} \int_A d^2 R_1 \ldots d^2 R_N \, \mathrm{Im}\left[\Psi^* \frac{\partial}{\partial z} \Psi\right] \tag{8}$$

where $\hbar = m = 1$ for brevity, and obtain after a lengthy but, in principle, simple calculation

$$\begin{aligned} \langle j_z \rangle = T(q_{0,l}) \mathrm{Re}[q_{0,r}] - \mathcal{N} \mathrm{Re}\bigg[& T(q_{0,l}) \frac{q_{0,r}}{q_{0,l}} \langle f \rangle [1 + r(q_{0,l})] \\ & - \langle |f|^2 \rangle |1 + r(q_{0,l})|^2 \int d^2 p \, \frac{q_r T(q_l)}{4q_l^2} \bigg] \end{aligned} \tag{9}$$

where the first term is the current density through the ideal barrier, and $T \equiv |t|^2$. Here, we have defined the averaged quantities $\langle f \rangle \equiv N^{-1} \sum_n f^{(n)}$ and $\langle |f|^2 \rangle \equiv N^{-1} \sum_n |f^{(n)}|^2$.

In the following, we will restrict ourselves to the simple case of a rectangular barrier with $v(z) = v$ although the barrier is biased. The more realistic case where the barrier potential is a trapezoid, $v(z) = v + (w/L)z$, due to a potential difference $eU = \hbar^2 w/2m$ across the barrier, is treated in the appendix, and it is shown there that the rectangular-barrier model gives a good approximation for reasonable potential drops [20]. Additionally, we assume that $L^2(v - k^2) \gg 1$, i.e. the tunnel effect is weak, and $v \gg k^2$, i.e. the particle energy is well below the barrier top. Then we have the following relations [21]:

$$r(q_l) = \frac{iq_l + \kappa}{iq_l - \kappa} \qquad T(q_l) = \frac{16\kappa^2 q_l^2}{v^2} e^{-2\kappa L} \tag{10}$$

with $\kappa^2 = v + p^2 - k^2$.

Formula (9) requires further analysis. For this purpose, we rewrite the term containing $\langle f \rangle$, using the first relation of (10) and the optical theorem [22]

$$\mathrm{Im} f = |f|^2 \mathrm{Im} G(r, r)_{z=0} = |f|^2 2\pi k^3 / 3v \tag{11}$$

where equation (7) has been employed for the second equality and the integration over p (see equation (4)) has been performed. From equation (11) we find that the term with $\mathrm{Im} f$ can be neglected in all further formulae since it is always small, of order k^2/v, according to the assumption made above. This is a peculiarity of the present tunnelling problem. In discussions on an isolated scatterer [23] this term plays an important role because it describes the interference of incident and scattered fields.

Now equation (9) reads

$$\langle j_z \rangle = T(q_{0,l}) \left(1 + \mathcal{N} \langle \mathrm{Re} f \rangle \frac{2\kappa}{v} \right) \mathrm{Re}[q_{0,r}] + \mathcal{N} \langle |f|^2 \rangle \mathrm{Re} \left[\frac{q_{0,l}^2}{v} \int \mathrm{d}^2 p \, \frac{q_r T(q_l)}{4 q_l^2} \right]. \tag{12}$$

First we consider the term proportional to $\langle \mathrm{Re} f \rangle$. From (10) we find that $(\mathrm{d}/\mathrm{d}L) T = -2\kappa T$, and thus we can interpret the $\langle \mathrm{Re} f \rangle$ term as a correction to the transmittivity $T(q_{0,l})$ due to a change in the effective barrier thickness:

$$T(q_{0,l}) \to T_{\mathrm{eff}}(q_{0,l}) = T(q_{0,l}) - \frac{\mathrm{d}T(q_{0,l})}{\mathrm{d}L} \frac{\mathcal{N} \langle \mathrm{Re} f \rangle}{v}. \tag{13}$$

If the characteristic bump dimensions are small compared to the penetration depth κ^{-1}, $\mathrm{Re} f \simeq f$ can be simply calculated by means of the Born approximation [22] $f \simeq \mathrm{Re} f \simeq vhb$, where h is the characteristic bump height and b the area on the surface occupied by the bump. (On the other hand, if the surface is covered with uncorrelated particles that can be treated as hard spheres with diameter a, $f \simeq -a$ holds.)

If convex and concave bumps occur with the same statistical weight, i.e. $\langle h \rangle = 0$, the effective thickness remains unchanged, of course. This first correction term changes neither the direction of the current flowing through the barrier nor the dependence of the current on the bias w compared to an ideal barrier. As for ideal barriers, the main flux through the barrier increases if $w < k^2 \cos^2 \varphi_0 = q_{0,l}^2$.

In contrast, the integral in the term proportional to $\langle |f|^2 \rangle$ corresponds to diffuse scattering of particles in all directions due to surface roughness. Particles incident on the barrier in a state p_0 are scattered into other states p. On the other hand, particles are allowed to tunnel if $w < k^2 - p^2$. Consequently, a current through the *rough* barrier is also possible in the bias range $q_{0,l}^2 \leqslant w \leqslant k^2$ made up of particles diffusely scattered into states with $p^2 < p_0^2$. This leads to a tail in the $\langle j_z \rangle$ versus w plot for non-perpendicular incidence, i.e. $\varphi_0 > 0$. This should be observable experimentally.

If the bias has crossed the onset point of the ideal barrier, i.e. $w < q_{0,l}^2$, the contributions due to diffuse scattering are outweighed by the main current due to the initial state with p_0.

For the case where convex and concave bumps are present with the same statistical weight, roughness always leads to enhanced transmission due to diffuse current contributions. This has already been shown to be true for disturbed barriers in [14], [16] and [13]. On the other hand, if the bumps are mainly vaulted outward, the total transmissivity of the barrier above the onset point $w = q_{0,l}^2$ is decreased as long as the correction to T_{eff} which is of first order in $\langle f \rangle$ outweighs the diffuse scattering term depending on $\langle |f|^2 \rangle$.

The integral in equation (12) can be solved approximately, taking into account the fact that the exponential of $T(q_l)$ is nearly constant in the integration range $p^2 \ll \sqrt{v}/L$. For $p^2 \gg \sqrt{v}/L$, the integral is cut off by this exponential. Thus, in the bias range of interest here, i.e. around the onset point of the ideal barrier, $k^2 \geqslant w \geqslant 0$, the total mean current density finally reads

$$\langle j_z \rangle \simeq T_{\mathrm{eff}}(q_{0,l})(q_{0,l}^2 - w)^{1/2} + \tfrac{2}{3}\pi \mathcal{N}\langle |f|^2 \rangle T(q_{0,l})(k^2 - w)^{3/2}/v. \tag{14}$$

We remark without explicit calculation that the same result is obtained if the rough side of the barrier is that at $z = L$.

In figure 2 is given a plot of $\langle j_z \rangle$ versus w around the onset point $q_{0,l}^2$ of the main current. The contribution of the diffuse scattering below the onset point can be easily seen.

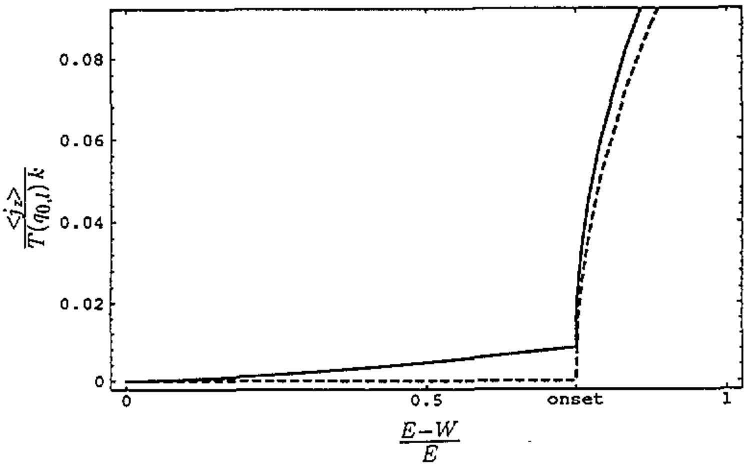

Figure 2. Solid line, plot of the mean current density passing through a rough barrier versus the (normalized) difference of particle energy E and bias W. The particles are incident under an angle $\varphi_0 = \pi/3$. The roughness parameters are $\langle \mathrm{Re} f \rangle = 0$, i.e. concave and convex bumps occur with the same weight, and $\mathcal{N}\langle |f|^2 \rangle = 0.5$. The ratio k^2/v is equal to 0.01, i.e. the particle energy is much smaller than the barrier potential. The tail due to diffuse scattering as well as the sharp onset of the main current are clearly seen. Broken line, barrier with the same parameters but without roughness.

The diffuse current contribution is proportional to the typical quantity $\mathcal{N}\langle |f|^2 \rangle$ related to the scattering picture of the present paper and can be seen as the product of a mean surface coverage factor $B \equiv \mathcal{N}b$ and h^2bv^2. This can be easily translated into the language employed by other authors [24] using the product of the surface height profile RMS Δ and correlation length ξ, as was shown in [6].

In order to make contact with a current experimental situation we relate the diffuse current density $\langle j_{\mathrm{diff}} \rangle$ just below the onset of the main current to that for zero bias $\langle j_{\mathrm{zero}} \rangle$ for an AlGaAs barrier. We suppose that $\langle f \rangle = 0$ and use typical barrier parameters from [25]. Electrons of energy 12 meV are incident under an angle of $\varphi_0 = \pi/4$ on the AlGaAs barrier with 120 meV height. The roughness parameters are those presented by Sakaki and co-workers [26], i.e. $h = 0.6$ nm and $b = 36$ nm^2. For the coverage factor we assume that $B = 0.4$. With these data we obtain $\langle j_{\mathrm{diff}} \rangle / \langle j_{\mathrm{zero}} \rangle = 0.2$. Thus roughness scattering in such a barrier leads to a measurable tail.

3. Generalization of equation (12)

Here, we will generalize the treatment given in the preceding section. The configurational average of j_z (which gives the mean current passing through the barrier) destroys all interferences of the scattered waves. Thus, the diffuse current density is the sum over all currents J_n^+ emerging from the bumps into the region $z > L$, multiplied by the mean bump density $\mathcal{N}$. J_n^+ is simply

$$\begin{aligned} J_n^+ &= |\phi_0(\boldsymbol{r}_n)|^2 |f^{(n)}|^2 \int_{z>L} \mathrm{d}^2 A \, \mathrm{Im}[G^*(\boldsymbol{r}, \boldsymbol{r}_n) \nabla G(\boldsymbol{r}, \boldsymbol{r}_n)] \\ &= |\phi_0(\boldsymbol{r}_n)|^2 |f^{(n)}|^2 \, \mathrm{Im} G^+(\boldsymbol{r}_n, \boldsymbol{r}_n) \end{aligned} \tag{15}$$

where $\mathrm{Im}G^+(\boldsymbol{r}_n, \boldsymbol{r}_n)$ contains only states that carry a current to $z > L$. Thus

$$\langle j_z \rangle \simeq T_{\mathrm{eff}}(q_{0,l}) \, \mathrm{Re}[q_{0,r}] + |\phi_0|^2 \mathcal{N} \langle |f|^2 \rangle \, \mathrm{Im} G^+. \tag{16}$$

$|\phi_0|^2$ and $\mathrm{Im}G^+$ must be taken at the rough side of the barrier. If both sides are rough, the corresponding contributions simply add.

Equation (9) provides a test of the general expression (16). Indeed, if we separate in $\mathrm{Im}G(\boldsymbol{r}, \boldsymbol{r})_{z=0}$ the states eventually giving a current into the region $z > L$ (see (7) and (6)) we can identify

$$\mathrm{Im}G^+ = \mathrm{Re}\left[\int \mathrm{d}^2 p \, \frac{q_r T(q_l)}{4 q_l^2} \right].$$

On the other hand, it is obvious that

$$|\phi_0|^2 = |1 + r(q_{0,l})|^2.$$

The generalized expression (16) turns out to be useful in cases where scattering is possible only into a discrete set of states, as for instance in quantum-well structures.

4. Conclusions

In this paper, the influence of surface roughness of a tunnel barrier on the current passing through has been investigated. The roughness was modelled by uniformly and uncorrelatedly distributed bumps.

The action of the roughness has been shown to be twofold. Firstly, the effective barrier width is changed according to the mean bump height and the surface fraction that is occupied by the perturbations. Secondly, the sharp rise of the current through an ideal barrier if the bias potential crosses the onset point is washed out in the presence of surface roughness. This is explained by elastic scattering of particles into states with higher normal component of the wave vector. The presence of roughness on the barrier always leads to an enhancement of the tunnelling current.

We have argued that the diffuse current density contributions can be expressed by a product of absolute squares of incident field and bump scattering amplitude, and the local density of states at the rough barrier surface. Seen from this point of view, formula (14) turns out to be a special case for a continuum of scattering states.

Finally, there is an essential point to mention. The results given here are obtained under the assumption of a single plane wave incident on the barrier under a well defined angle. This corresponds to an experimental situation similar to that of photon tunnelling [17, 18]. Information about the roughness parameters can be gained by measuring the fraction of diffusely scattered particles. On the other hand, in the case of a bulk material, a continuum of incidence angles is possible. Therefore the current tail discussed here will not be observable. In contrast, in the case of tunnelling from a quantum well where only a few lateral modes are occupied, it should be possible to detect the lateral modes as well as the tail by tunnelling spectroscopy (TS). Structures that seem to be appropriate have been proposed in [27] and [28]. TS experiments on quantum structures have already been carried out [29–31]. Thus, TS on quantum structures could provide a tool for the estimation of surface roughness.

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Appendix

Consider a barrier potential profile

$$v(z) = v + Fz \qquad F \equiv w/L. \tag{A1}$$

The differential equation (5) with a barrier potential (A1) has in the barrier region $0 \leqslant z \leqslant L$ solutions that are called Airy functions [32, 22]. They can be expressed as

$$\Phi_+(z) = a\sqrt{\xi}K_{1/3}(\tfrac{2}{3}\xi^{3/2}) \qquad \Phi_-(z) = b\sqrt{\xi}I_{1/3}(\tfrac{2}{3}\xi^{3/2}) \tag{A2}$$

where the dimensionless variable $\xi \equiv F^{1/3}(z + \kappa^2/F)$ has been defined for the sake of brevity. $K_{1/3}$ and $I_{1/3}$ are the so-called modified Bessel functions. $\Phi_\pm(\xi)$ correspond to the solutions $e^{\mp\kappa z}$ inside a rectangular barrier.

The $\Phi_\pm(z)$ have to be matched to the oscillating solutions outside the barrier by an appropriate choice of the coefficients a and b according to the matching conditions

$$\begin{aligned} 1 + r(q_l) &= \Phi_+(0) + \Phi_-(0) \qquad & \mathrm{i}q_l[1 - r(q_l)] &= \left(\frac{\partial}{\partial z}\right)_{z=0} [\Phi_+(z) + \Phi_-(z)] \\ t(q_l)\mathrm{e}^{\mathrm{i}q_r L} &= \Phi_+(L) + \Phi_-(L) \qquad & \mathrm{i}q_r t(q_l)\mathrm{e}^{\mathrm{i}q_r L} &= \left(\frac{\partial}{\partial z}\right)_{z=L} [\Phi_+(z) + \Phi_-(z)]. \end{aligned} \tag{A3}$$

As in section 2, $w \ll v$ is assumed. This is equivalent to the condition $\xi \gg 1$, and thus we can use the asymptotic forms of $\Phi_\pm$

$$\Phi_\pm(z) \sim \xi^{-1/4}\exp(\pm\tfrac{2}{3}\xi^{3/2}). \tag{A4}$$

Inserting the asymptotic forms (A4) into the matching conditions (A3), we obtain

$$\begin{aligned} r(q_l) &\simeq \frac{\mathrm{i}q_l + \kappa[1 + F^{4/3}/4\kappa^4]}{\mathrm{i}q_l - \kappa[1 + F^{4/3}/4\kappa^4]} \\ T(q_l) &\simeq \frac{16\kappa^2 q_l^2}{v^2} \exp\left(-2\kappa L\left[1 + \frac{w}{4\kappa^2}\right]\right) \end{aligned} \tag{A5}$$

where only the largest correction term is included. (The approximation given here agrees with the result obtained by means of the WKB method used in [19].) Thus, under the assumptions made above, the saw-tooth barrier shape changes the results obtained for a rectangular barrier only slightly.

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