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Barrier penetration and Klein paradox

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Abstract. Particle penetration through a square potential barrier is studied with the Dirac equation and relativistic tunnelling occurs in an overcritical potential. Relations between this phenomenon and the Klein paradox are discussed. However, relativistic correction to the mesoscopic conduction, the Landauer formula, is negligible and relativistic tunnelling would not occur in solid-state physics owing to the barrier height never reaching the over-critical region. Relativistic tunnelling is essentially a high-energy phenomenon.

Barrier penetration is an important problem in scattering theory [1] and provides theoretical models for a variety of phenomena, e.g. tunnelling in Esaki diodes and quantum wells [2], alpha decay [3], quarkonium confinement [4], etc. In high-energy physics, application of the Dirac equation leads to the Klein paradox, which gives transmission probabilities different (strikingly larger) from the solutions of the Schrödinger equation under the overcritical scattering potential condition [5]. The Klein paradox can be explained by hole theory [4, 6]. The prediction of Dirac's theory on the vacuum change in supercritical fields has been verified by experiments [4, 6]. Hence, it is desirable to find a solution of the Dirac equation for a general square barrier and check its differences from that of the Schrödinger equation. In this paper we take the Landauer formula of mesoscopic conduction as an example.

The electrical-conductivity behaviour of ordinary metals has been studied extensively based on successive theoretical models and is thought to be well understood. The quantized free electron theory of metallic conduction concentrates on electron distribution changes resulting from acceleration by an applied electrical field and deceleration by scattering centres. The electrical conductivity can also be studied with the Kubo formula based on the linear response theory [7], in which the applied field is the causative agent and the resulting current flow the response. The traditional description of conductivity is challenged by the onset of strong-disorder (localization of electrons) and miniaturization of electronic devices. The unusual properties of wave phenomena in disordered media have been observed in submicron structures at low temperature, in which the electron wavefunctions maintain their quantum mechanical phase coherence. Hence, electron transport has to be studied in terms of transmission coefficients and electron waveguides rather than of the Boltzmann transport equation. Landauer proposed this novel point of view and related the conductance of a quantum

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mechanical system to scattering problems [8–10]. The Landauer formula

$$R_e = \frac{h}{e^2}\frac{R}{1-R} = \frac{h}{e^2}\frac{1-T}{T} \tag{1}$$

where R_e is the resistance and R and T are the reflection and transmission coefficients respectively, plays an important role in mesoscopic physics. It was derived for a strictly one-dimensional geometry and was later extended by Büttiker *et al* to the multiprobe and multichannel disordered system so as to compare with experimental work on quantum transport phenomena (e.g. [11]).

In this paper the relativistic extension of the Landauer formula is studied. The relativistic effect, though weak and covered by other effects in general, may come to the fore when contributions of other mechanisms vanish or cancel each other as in the ground-state splitting of S-state ions, e.g. Gd^{3+} and Mn^{2+} [12]. It might modify well known phenomenon, e.g. the interference pattern of the Aharonov–Bohm effect of relativistic particles with spin could be affected if the initial particle beam is polarized [13, 14]. It may also produce new phenomena such as the positron predicted by Dirac's theory. All these, together with the Klein paradox, make us interested in finding any new results from the application of Dirac's theory to the Landauer formula.

Following Landauer's derivation [8], the resistance of a one-dimensional conductor sandwiched between two phase-randomizing reservoirs (where all the dissipation occurs) is

$$R_e = \frac{2R}{1-R}\frac{\partial\mu/\partial n}{e^2 v_F} \tag{2}$$

where μ is the chemical potential (equal to the Fermi energy at 0 K), n the electron density and v_F the Fermi velocity. In the relativistic case, the particle number density n is

$$n = 2p_F/\pi\hbar \tag{3}$$

for one-dimensional Fermi gas where p_F is the Fermi momentum, and the Fermi energy

$$\mu^2 = \mathscr{E}_F^2 = p_F^2 + m^2 = (\pi\hbar n/2)^2 + m^2 \tag{4}$$

where m is the rest mass of the electron and c is taken to be 1. Substituting equation (4) into equation (2) we obtain

$$R_e = (\pi\hbar/e^2)(R/T)m/[(\pi\hbar n/2)^2 + m^2]^{1/2}. \tag{5}$$

This is the relativistic extension of the Landauer formula. The relativistic correction (RC) can be estimated from

$$[1 + (\pi\hbar n/2mc)^2]^{-1/2} \simeq 1 - (1/8)(\pi\hbar h n/mc)^2$$

in the first-order approximation. The second term is only about 0.06% if n is taken as the cube root of the gold electron concentration ($5.8\times10^{28}\,m^{-3}$). RC is negligible and usually, $(\pi\hbar n/2)^2 \ll m^2$ is satisfied. Equation (5) reduces to equation (1) in the non-relativistic limit.

However, the relativistic effect also shows in the transmission behaviour of low-energy electrons. Let us consider a sandwich device shown in figure 1, where regions I and III are ideal leads separately connect to two incoherent reservoirs, and II is the disordered region, as an obstacle, represented by a square barrier potential of height

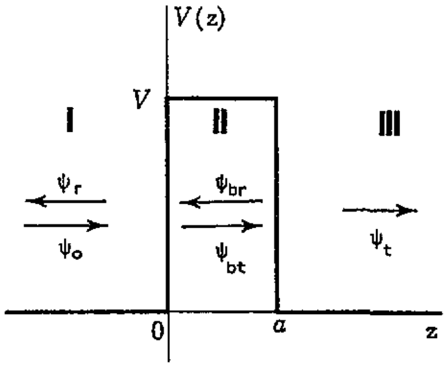

Figure 1. A one-dimensional square potential barrier of height V and width a.

V in $[0, a]$. Figure 1 is just the Landauer situation in which a stream of electrons (in the region $z<0$) with unit density are incident upon the potential barrier in the direction of the z-axis. A fraction R is reflected and a fraction T transmitted. The plane-wave functions in various regions are

$$\psi_0=\begin{bmatrix}1\\0\\k/(m+E)\\0\end{bmatrix}e^{ikz} \qquad \psi_r=r\begin{bmatrix}1\\0\\-k/(m+E)\\0\end{bmatrix}e^{-kz} \qquad \text{(region I)}$$

$$\psi_{bt}=b_1\begin{bmatrix}1\\0\\k_1/(m+E-V)\\0\end{bmatrix}e^{ik_1z} \qquad \psi_{br}=b_2\begin{bmatrix}1\\0\\-k_1/(m+E-V)\\0\end{bmatrix}e^{-ik_1z} \qquad \text{(region II)}$$

$$\psi_t=t\begin{bmatrix}1\\0\\k/(m+E)\\0\end{bmatrix}e^{ikz} \qquad \text{(region III)} \tag{6}$$

in unit system with $\hbar=1, c=1$, where the subscripts 0, r, t and b are for incident, reflected, transmitted and barrier respectively, k and k_1 are electron momenta outside and within the barrier respectively

$$E^2=m^2+k^2 \tag{7}$$

$$(E-V)^2=m^2+k_1^2. \tag{8}$$

The spin orientation does not affect the results of barrier penetration and here only the spin-up electron is considered. Boundary conditions at $z=0$ and a lead to

$$1+r=b_1+b_2 \qquad k(1-r)/(m+E)=k_1(b_1-b_2)/(m+E-V)$$

$$t\,e^{ika}=b_1\,e^{ik_1a}+b_2\,e^{ik_1a} \qquad tk\,e^{ika}/(m+E)=k_1(b_1\,e^{ik_1a}-b_2\,e^{-ik_1a})/(m+E-V)$$

which can be expressed in a matrix form

$$\begin{bmatrix} 1 & 0 & -1 & -1 \\ -k/(m+E) & 0 & -k_1/(m+E-V) & k_1/(m+E-V) \\ 0 & e^{ika} & -e^{ik_1a} & -e^{-ik_1a} \\ 0 & k\,e^{ika}/(m+E) & -k_1\,e^{ik_1a}/(m+E-V) & k_1\,e^{-ik_1a}/(m+E-V) \end{bmatrix} \begin{bmatrix} r \\ t \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} -1 \\ -k/(m+E) \\ 0 \\ 0 \end{bmatrix}. \tag{9}$$

R and T are obtained by solving equation (9)

$$\begin{aligned} R &= |r|^2 = m^2V^2\sin^2(k_1a)/[(k_1k\cos(k_1a))^2+(E^2-m^2-EV)^2\sin^2(k_1a)] \\ &= (mV/k_1k)^2\sin^2(k_1a)/[1+(mV/k_1k)^2\sin^2(k_1a)] \end{aligned} \tag{10}$$

$$\begin{aligned} T &= |t|^2 = k_1^2k^2/[(k_1k\cos(k_1a))^2+(E^2-m^2-EV)^2\sin^2(k_1a)] \\ &= 1/[1+(mV/k_1k)^2\sin^2(k_1a)] \end{aligned} \tag{11}$$

and they satisfy $R+T=1$. In the non-relativistic limit, $k^2=2mE$ and $k_1^2=2m(E-V)$ so that equation (11) reduces to

$$T_s = \{1+[V^2/4E(E-V)]\sin^2[a\sqrt{2m(E-V)}]\}^{-1} \tag{12}$$

which is in agreement with that from the Schrödinger equation (e.g. [15]).

The transmission amplitude of equation (11) has remarkably different behaviour from that of equation (12) when the barrier height V approaches the critical potential, defined as $V_c=E+m$. Taking an extreme case of $V\to\infty$, it can be seen that the behaviours of barrier tunnelling based on non-relativistic and relativistic physics are essentially opposite. Equation (12) predicts $T_s\to 0$ when $V\to\infty$ and hence, $R_e\to\infty$. A Schrödinger particle cannot penetrate an infinite barrier, as shown in figure 1(*b*) of [15]. However, since

$$\lim_{V\to\infty}[mV/(k_1k)]^2 = m^2/(E^2-m^2)$$

then

$$T \xrightarrow[V\to\infty]{} [1+m^2\sin^2(k_1a)/(E^2-m^2)] \tag{13}$$

based on equation (11), and hence low-energy Dirac particles can penetrate a barrier of infinite height. Furthermore, if $k_1a=l\pi$ $(l=0,1,2,3,\ldots)$, T becomes one and relativistic tunnelling occurs. Correspondingly, the resistance

$$R_e = (\hbar\pi/e^2)[m^2\sin^2(k_1a)/(E^2-m^2)]\{m/[(n\pi\hbar/2)^2+m^2]\} \tag{14}$$

when $V\to\infty$ and $R_e=0$ in relativistic tunnelling.

The relativistic tunnelling can be understood by the Klein-paradox explanation [5-6]. With the critical potential, the energies of the electron level spectrum within the barrier region are lifted by V and the occupied lower-energy states continuum (in the energy region smaller than $V-m$) 'outcrop', which overlaps a part of the positive-energy spectrum outside the barrier. Incident electrons impact onto the potential barrier and can thus knock out electrons from these states inside the barrier so as to induce electron–positron pair-production at the barrier. Then there are positron waves inside the barrier and resonance penetration occurs. The relativistic tunnelling is associated with induced decay of vacuum in overcritical fields. Application of a supercritical field changes the Dirac vacuum, and thus drastically alters the characteristics of sample including its resistance, which originates from the same mechanism of the Klein paradox.

However, the discovery of relativistic tunnelling does not mean failure of insulation in microelectronics since, in solid-state physics, the barrier height (representing a mesoscopic scattering region) is only in the order of 10 eV but the critical potential in the order of 1 MeV. Relativistic tunnelling would not occur in solid-state conduction even though inappropriate use of 'infinite barrier height' is frequently seen. On the contrary, it is a high energy phenomenon and plays an important role in quarkonium confinement [4].

In summary, the problem of particle (electron) penetration through a square potential barrier is solved with the Dirac equation. It is found that the transmission coefficient can be equal to one even when the barrier height tends to infinity. This striking phenomenon is named relativistic tunnelling and can be understood on the basis of the Klein paradox. However, relativistic tunnelling only occurs in the high-energy region (barrier height ~ MeV) and for solid-state conduction, solutions of the Schrödinger equation are enough for interpreting experiments.

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