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Adiabaticity in quantum transport

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Abstract. It is commonly assumed that electrons evolve adiabatically in quantum transport devices, and so remain in the same transverse quantum state throughout the system. This model simplifies the analysis of such devices and the model correctly predicts that the conductance of a system containing a number of constrictions is quantised with a value equal to the conductance of the narrowest constriction. In this paper the validity of the adiabatic model for the evolution of the electronic wavefunctions is investigated via an analysis of the behaviour of a wavefunction in a one-dimensional potential well whose width increases with time. It is found that the evolution becomes strongly non-adiabatic no matter how small the rate of increase in the width of the well. This invalidates the previous interpretation of the origin of a quantised conductance in devices containing several constrictions. However, it is shown that the quantisation of the conductance in these devices can be explained by replacing the requirement of adiabaticity in the evolution of the transverse electronic wavefunctions with the requirement of reversibility.

1. Introduction

There has recently been a considerable increase in interest in the subject of quantum transport following the successful fabrication of devices that show quantised conductances attributable to quantum transport (van Wees *et al* 1988, Wharam *et al* 1988b). Theoretical studies of the origin of the quantised conductance in devices that contain a single narrow contriction have been presented by several authors (Landauer 1988, Widom and Tao 1988, Szafer and Stone 1989). Experiments on systems that contain more than one constriction show that the conductance of these devices is also quantised and is equal to the conductance of the narrowest constriction (Wharam *et al* 1988a). This result is easily explained by assuming that the electronic wavefunctions evolve adiabatically in the device so that the electrons remain in the same transverse quantum state throughout the system (Beenakker and van Houten 1988). In this case any electron that can propagate through the narrowest constriction can pass through every other constriction because the energy in the transverse direction in these constrictions is smaller than it was in the narrowest constriction and so the longitudinal energy of the electron remains positive throughout the device. Landauer has used the assumption of adiabatic evolution of the wavefunctions to analyse the conductance of devices that contain a single contriction (Landauer 1988). In this work Landauer was primarily concerned with the effect of self-consistency on the conductance of the device and the assumption of adiabatic evolution of the wavefunctions was used to simplify the analysis. Szafer and Stone (1989) have calculated the conductances of a number of devices that

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contain narrow constrictions. They have shown that there is no significant variation between the conductance of a device in which the change in the width of the channel is abrupt and the conductance of a device in which the width of the channel changes gradually to give a greater degree of adiabaticity in the evolution of the electronic wavefunctions. Therefore the conductance of devices that contain single constrictions appears to be relatively insensitive to the degree of adiabaticity in the evolution of the electronic wavefunctions. This suggests that Landauer's conclusions concerning the conductance of devices that contain single constrictions can be applied to any such device independently of the degree of adiabaticity in the evolution of the electronic wavefunctions. The reason for the relative insensitivity of the quantisation of the conductance to the degree of adiabaticity in the evolution of the electronic wavefunctions in these devices is discussed briefly in § 3.

An investigation of the validity of the adiabatic model for the evolution of the electronic wavefunctions in quantum transport devices is presented in the following section. The evolution of a wavefunction in a one-dimensional potential well whose width varies with time is analysed and it is found that the evolution of the wavefunction becomes strongly non-adiabatic no matter how small the rate of increase in the width of the well. This invalidates the simple model for the quantisation of the conductance in devices that contain several constrictions because the electrons will not remain in the same transverse quantum states throughout the system. However, the quantisation of the conductance in these devices requires the less stringent condition of reversibility in the evolution of the transverse wavefunctions to ensure that the electronic wavefunction returns to the same transverse quantum state in each of the constrictions. In § 3 it is shown that the condition for reversibility in the evolution of the transverse electronic wavefunctions is not strongly violated, so the conductance of devices that contain several narrow constrictions will be quantised.

The systems investigated experimentally have a two-dimensional geometry but the evolution of the wavefunction in the transverse direction can be approximately analysed using the one-dimensional model adopted in this paper by computing the width of the potential well at time t from the geometry of the system and the longitudinal velocity of the electron. The complications that arise from the two-dimensional geometry are briefly discussed in § 3.

2. Evolution of a wavefunction in a one-dimensional time-dependent potential well

The wavefunction of an electron in a one-dimensional potential well whose width varies with time can be written as a superposition of the instantaneous eigenstates of the system. In this paper it will be assumed that the origin of coordinates lies at the centre of the potential well and that the potential well remains symmetric about this point. In this case the symmetry of the initial wavefunction will be conserved during the expansion of the well. For convenience it will be assumed that the initial electronic state is symmetric so that only the symmetric eigenstates have to be included in the expansion of the wavefunction. The wavefunction at time t can be written as

$$\psi(t) = \sum_n c_n(t) \frac{1}{w(t)^{1/2}} \cos\left(\frac{(2n+1)\pi x}{w(t)}\right) \tag{1}$$

where $w(t)$ is the width of the potential well at time t.

Substituting this expression into the time-dependent Schrödinger equation gives

$$i\hbar \sum_n \dot{c}_n(t) \frac{1}{w(t)^{1/2}} \cos\left(\frac{(2n+1)\pi x}{w(t)}\right) + i\hbar \sum_n c_n(t) \frac{-\frac{1}{2}\dot{w}(t)}{w(t)^{3/2}} \cos\left(\frac{(2n+1)\pi x}{w(t)}\right)$$

$$+ i\hbar \sum_n c_n(t) \frac{1}{w(t)^{1/2}} \frac{(2n+1)\pi x \dot{w}(t)}{w(t)^2} \sin\left(\frac{(2n+1)\pi x}{w(t)}\right)$$

$$= \sum_n \frac{\hbar^2 (2n+1)^2 \pi^2}{2mw(t)^2} c_n(t) \frac{1}{w(t)^{1/2}} \cos\left(\frac{(2n+1)\pi x}{w(t)}\right) \tag{2}$$

where m is the electronic mass.

The equation of motion for the coefficient c_n is

$$\dot{c}_n(t) = \frac{\hbar(2n+1)^2\pi^2}{2imw(t)^2} c_n(t) - \sum_{p \neq n} c_p(t)$$

$$\times \frac{(2p+1)\pi x \dot{w}(t)}{w(t)^3} \int_{-w(t)/2}^{w(t)/2} \cos\left(\frac{(2n+1)\pi x}{w(t)}\right) \sin\left(\frac{(2p+1)\pi x}{w(t)}\right) x \, dx. \tag{3}$$

The second term in (2) cancels with the diagonal component of the third term when deriving (3).

Two particular forms for $w(t)$ will be considered, a linear variation with time and a quadratic variation with time. The evolution of the wavefunction in a widening potential well rather than a narrowing well will be considered for reasons that become apparent later.

In the case of a linear variation of the width of the well with time the equations of motion for the coefficients c_n can be simplified by using the following expression for the wavefunction:

$$\psi(t) = \sum_n c_n(t) \frac{1}{(a+vt)^{1/2}} \cos\left(\frac{(2n+1)\pi x}{a+vt}\right) \exp\left(\frac{i\hbar (2n+1)^2 \pi^2}{2mv(a+vt)}\right) \tag{4}$$

where a is the initial width of the potential well and v is the rate of increase in the width of the well.

Substituting (4) into the Schrödinger equation gives the equations of motion for the coefficients c_n as

$$\dot{c}_n(t) = -\sum_{p \neq n} c_p(t) \frac{(2p+1)\pi v}{(a+vt)^3} \exp\left(\frac{2i\hbar(p^2+p-n^2-n)\pi^2}{mv(a+vt)}\right)$$

$$\times \int_{-(a+vt)/2}^{(a+vt)/2} \cos\left(\frac{(2n+1)\pi x}{a+vt}\right) \sin\left(\frac{(2p+1)\pi x}{a+vt}\right) x \, dx. \tag{5}$$

This set of coupled equations can be considerably simplified by working in the Born approximation and by assuming that the wavefunction is initially an instantaneous eigenstate of the system—here it will be assumed that it is the lowest-energy eigenstate. Since only first-order terms are retained in the Born approximation the value of the

coefficient c_0 remains equal to 1 and, to first order, the equations of motion for the coefficients c_n can be written as

$$\dot{c}_n(t) = -[\pi v/(a+vt)]M(n)\exp[-2i\hbar(n^2+n)\pi^2/mv(a+vt)] \qquad n \neq 0 \tag{6}$$

where

$$M(n) = \int_{-1/2}^{1/2} \cos[(2n+1)\pi x]\sin(\pi x)x\,\mathrm{d}x \tag{7}$$

which gives

$$c_n(t) = -\pi v M(n)\int_0^t \frac{\exp[-2i\hbar(n^2+n)\pi^2/mv(a+vt')]}{(a+vt')}\,\mathrm{d}t' \qquad n \neq 0. \tag{8}$$

The variation in the magnitudes of the coefficients depends on the value of $2\hbar(n^2+n)\pi^2/mv(a+vt)$. For times t such that $2\hbar(n^2+n)\pi^2/mv(a+vt) \gg \pi$ the phase factor in the integral is rapidly varying and the amplitude of c_n remains small. When $2\hbar(n^2+n)\pi^2/mv(a+vt) \ll \pi$ the phase factor is effectively independent of time and the value of $c_n(t)$ is given by

$$c_n(t) = -\pi M(n)\ln\{(a+vt)/[2\pi^2\hbar(n^2+n)/mv]\}. \tag{9}$$

The values of all the coefficients c_n are unbounded no matter how small the rate of increase in the width of the channel with time. The non-adiabicity arises because the difference between the energies of the first and any higher quantum state decreases as the potential well widens, at some point the perturbation due to the increase in the width of the well is large compared with the energy difference between the states and the condition for the adiabatic evolution of the wavefunction is violated. The neglect of second- and higher-order terms in (6) is responsible for the continuous increase in the magnitudes of the coefficients and including these terms in the equations of motion will ensure that the wavefunction remains normalised. However, the higher-order terms in the equations of motion will only affect the evolution of the wavefunction when a significant weight of the wavefunction is in higher quantum states, so adding these terms to the equations of motion will not change the conclusion concerning the non-adiabicity of the evolution of the wavefunction.

The evolution of the electronic wavefunction in a one-dimensional potential well whose width increases quadratically with time will now be investigated. The width of the well at time t will be taken to be $a + bt^2$. In this case the equations of motion for the coefficients c_n can be simplified by choosing the following expression for the wavefunction:

$$\psi(t) = \sum_n c_n(t)\frac{1}{(a+bt^2)^{1/2}}\cos\left(\frac{(2n+1)\pi x}{a+bt^2}\right) \times \exp\left[\left[\frac{i\hbar(2n+1)^2\pi^2}{4ma}\left\{\frac{t}{a+bt^2} + \frac{1}{(ab)^{1/2}}\tan^{-1}\left[\left(\frac{b}{a}\right)^{1/2}t\right]\right\}\right]\right]. \tag{10}$$

The equations of motion for the coefficients c_n are then given by

$$\dot{c}_n(t) = \sum_{p\neq n} c_p(t)\frac{2(2p+1)\pi bt}{a+bt^2}\int_{-(a+bt^2)/2}^{(a+bt^2)/2}\cos\left(\frac{(2n+1)\pi x}{a+bt^2}\right)\sin\left(\frac{(2p+1)\pi x}{a+bt^2}\right)x\,\mathrm{d}x \times \exp\left[\left[\frac{i\hbar(p^2+p-n^2-n)}{ma}\left\{\frac{t}{a+bt^2} + \frac{1}{(ab)^{1/2}}\tan^{-1}\left[\left(\frac{b}{a}\right)^{1/2}t\right]\right\}\right]\right]. \tag{11}$$

Applying the Born approximation and assuming the initial wavefunction is the lowest-energy eigenstate of the instantaneous Hamiltonian gives the coefficients at time t as

$$c_n(t) = -2\pi bM(n)\int_0^t \frac{t'}{a+bt'^2}\exp\left[\frac{-i\hbar(n^2+n)\pi^2}{ma}\left\{\frac{t'}{a+bt'^2} + \frac{1}{(ab)^{1/2}}\tan^{-1}\left[\left(\frac{b}{a}\right)^{1/2}t'\right]\right\}\right]dt' \qquad n \neq 0. \tag{12}$$

The amplitudes of the coefficients remain small for times t such that the inequality $\hbar(n^2+n)\pi^2 t/ma(a+bt^2) \gg \pi$ holds, but for large values of t when $\hbar(n^2+n)\pi^2 t/ma(a+bt^2) \ll \pi$ the value of each coefficient increases continuously and is

$$c_n(t) = -2\pi M(n)\exp\left(\frac{-i\hbar(n^2+n)\pi^3}{2ma(ab)^{1/2}}\right)\ln\left(\frac{a+bt^2}{[a+\hbar^2(n^2+n)^2\pi^4/bm^2a^2]}\right) \qquad n \neq 0. \tag{13}$$

The evolution of the electronic wavefunction is again highly non-adiabatic although this is less surprising than in the previous example because in this example the magnitude of the perturbation increases with time since the rate of change of the width of the well increases with time. The examples considered in this section show that the transverse wavefunction of an electron in a quantum transport device cannot evolve adiabatically in a continuously widening channel no matter how slowly the width of the channel increases.

2. Non-adiabaticity and quantisation of the conductance

The effects of non-adiabaticity in the evolution of the transverse electronic wavefunctions in quantum transport devices will be discussed in this section. The effect of non-adiabaticity on the quantisation of the conductance in a device that contains a single constriction will be considered first. It will be assumed that only electrons in the lowest transverse quantum state can pass through the constriction. An electron in the lowest transverse quantum state *approaching* the constriction from the wide region of the device will be strongly scattered to higher quantum states as soon as the channel begins to narrow. Providing that a particular higher quantum state is occupied the scattering from the lowest quantum state to this higher state will be exactly compensated by scattering in the opposite direction so the occupancy of these quantum states is not changed. It is only the scattering from the lowest transverse quantum state to unoccupied states that reduces the occupancy of the lowest state and destroys the quantisation of the conductance. The magnitude of the scattering from the lowest state to the unoccupied states is very small due to the large difference between the transverse energies of the states. Although the evolution of the transverse electronic wavefunction is strongly non-adiabatic in the widest regions of the device the non-adiabaticity will not destroy the quantisation of the conductance providing that in these regions a large number of transverse quantum states are occupied in the range of energies of the current-carrying states. Closer to the constriction the width of the channel is greatly reduced and the spacing between the energies of the transverse quantum states increases. Consequently the evolution of the wavefunctions becomes more adiabatic towards the constriction and the electrons will pass adiabatically through the narrowest regions of the device as long as there are no abrupt changes in the width of the channel.

Non-adiabatic evolution of the wavefunctions has a significant effect on the quantisation of the conductance in a device that contains a number of constrictions. Scattering from an occupied quantum state to a second quantum state cannot be compensated by scattering in the opposite direction if the second quantum state is unoccupied. In the region between the constrictions the majority of the transverse quantum states are unoccupied in the range of energies of the current-carrying states. Hence, the scattering from the lowest quantum state to higher quantum states in this region will not be compensated by scattering in the opposite direction. There will always be a significant scattering to higher transverse quantum states in a device in which the width of channel increases continuously and this might be expected to destroy the quantisation of the conductance in the device. However, this analysis has ignored the evolution of the wavefunction as the electron approaches the second constriction. Consider a device in which the two constrictions are of equal width. If only electrons in the lowest transverse quantum state can pass through the constrictions an electron will pass through the second constriction as long as its wavefunction evolves to the lowest transverse quantum state at the narrowest point in the second constriction. The electron must be in the lowest transverse quantum state to pass through the first constriction but it does not have to be in the lowest transverse quantum state at all points in between the constrictions in order to pass through the second constriction. The electron passing through the second constriction corresponds to the wavefunction in a one-dimensional potential well returning to its initial state when the width of the well has been reduced back to its initial value. One way of ensuring that an electron evolves to the lowest eigenstate of the instantaneous Hamiltonian in a one-dimensional potential well whose width decreases with time is to choose the initial state to be the time-reversed form of the wavefunctions calculated in the previous section. These wavefunctions evolved from the lowest-energy eigenstate of the instantaneous Hamiltonian as the width of the potential well increased and so the time-reversed wavefunctions will evolve to the lowest-energy eigenstate of the instantaneous Hamiltonian as the width of the potential well decreases to its initial value. If the width of the potential well is $a + v(2t' - t)$ or $a + b[(2t' - t)^2]$ for the period $t' < t < 2t'$, depending on whether the size of the well was increased linearly or quadratically, and the wavefunction at time t' is chosen to be $\psi^*(t')$, where $\psi(t')$ is the wavefunction that the lowest eigenstate of the initial Hamiltonian evolved to after time t', the wavefunction at time $2t'$ will be the lowest eigenstate of the instantaneous Hamiltonian. Therefore, the extent to which the electronic wavefunction evolves back to the lowest eigenstate in the one-dimensional system studied in the previous section is determined by the overlap between $\psi(t')$ and $\psi^*(t')$.

The degree of reversibility in the evolution of the wavefunction in a one-dimensional system is determined by the overlap between $\psi(t')$ and $\psi^*(t')$ which depends on the relative phases of the components of the wavefunction in different quantum states. If all the components are in phase the magnitude of the overlap is equal to 1 but it reduces as the phase differences increase. It is easiest to determine the overlap between $\psi(t')$ and $\psi^*(t')$ for the first example presented in the previous section because the phase factors in (4) are negligible for $t \gg 2\hbar(n^2 + n)\pi^2/mv^2$ and as the matrix elements $M(n)$ are real the relative phases of the components of the wavefunction in different quantum states are determined solely by the coefficients, c_n. From (9) it can be seen that the unbounded contributions to the coefficients are all real, so these components of the wavefunction are in phase. These contributions to the coefficients will vanish when the width of the well has been reduced to its initial value and only the imaginary parts of the coefficients will be non-zero. The degree of irreversibility in the evolution of the wavefunction is

determined by the imaginary parts of the coefficients at time $2t'$, which will be twice as large as their values at time t'. It can be concluded that the largest contribution to the non-adiabaticity in the evolution of the wavefunction is reversible and it does not prevent the wavefunction from returning to the lowest eigenstate of the instantaneous Hamiltonian when the width of the well has been reduced back to its initial value. Combining (14) with the phase factor in (10) for the case of the potential well whose width increases quadratically with time shows that the unbounded components of the wavefunction are all in phase so the conclusion about the degree of reversibility in the evolution of the wavefunction applies equally to this example. These results suggest that the conductance of a device that contains several constrictions will be accurately quantised because the evolution of the transverse wavefunctions is almost reversible.

The evolution of the transverse wavefunctions in the two-dimensional systems studied experimentally is less reversible than in the one-dimensional system investigated in this paper. Consider a device that contains two constrictions of equal width. If only electrons in the lowest transverse quantum state can pass through the constrictions the time-reversed solution to the Schrödinger equation for an electron in the region between the constrictions describes a wave packet that propagates to the lowest transverse quantum state in the first constriction. If the system has reflection symmetry in a line normal to and bisecting the line joining the two constrictions the time-reversed wavefunction can be reflected in this line to produce a wave packet that propagates to the lowest transverse quantum state in the second constriction. Hence, the amplitude of the wavefunction that propagates through the second constriction is determined by the overlap between ψ and the reflection of ψ^* in the line normal to and bisecting the line connecting the two constrictions. The degree of reversibility in the evolution of the wavefunction is now determined by the relative phases of the components of the wavefunction in different transverse quantum states and the spatial separation between the components, which arises because the components of the wavefunction in different transverse quantum states have different group velocities. After a time t_C given by

$$t_C = v\tau/\Delta v \tag{14}$$

where v is the average group velocity of the components of the wavefunction, τ is the coherence time of the initial wave packet and Δv is the smallest difference between the group velocities of any two components of the wavefunction, the electronic wavefunction will have separated into a set of discrete wave packets each wave packet containing the components of the wavefunction in a particular transverse quantum state. After this time the scattering between the quantum states that occurs when the channel narrows towards the second constriction cannot cancel the scattering that occurred when the width of the channel increased after the first constriction because of the spatial separation between the components of the wavefunction. The amplitude of the wavefunction that propagates through the second constriction will then be determined by the degree of adiabaticity in the evolution of the wavefunction rather than the degree of reversibility and the conductance will be smaller than its quantised value. The conductance will decrease continuously between its quantised value and this smaller value for times $0 < t < t_C$ but will remain at the smaller value for times greater than t_C.

4. Summary

It has been shown that the evolution of an electronic wavefunction in a potential well whose width increases with time becomes strongly non-adiabatic no matter how small

the rate of change in the width of the well. This invalidates the assumption of adiabatic evolution of the transverse wavefunctions which is often applied to quantum transport devices. The quantisation of the conductance in a device that contains a number of constrictions requires reversibility in the the evolution of the transverse electronic wavefunction rather than adiabaticity and it has been shown this condition is not strongly violated.

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