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Tranverse Scattering Resonances in Quantum Wires

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A theory for the effect of scattering by impurities in a quantum wire or electron waveguide is described. Scattering is strongly influenced by resonances which occur when a new mode of propagation appears as the Fermi energy is increased. These resonances can either increase or decrease the probability of backscattering by many orders of magnitude.

Es wird eine Theorie für die Auswirkung der Streuung an Unreinheiten in einem Quantendraht oder Elektronenwellenleiter beschrieben. Die Streuung wird stark durch die bei Anwachsen der Fermienergie neu auftretenden Ausbreitungsmoden beeinflußt. Diese Resonanzen können die Rückstreuung um mehrere Größenordnungen anwachsen oder abnehmen lassen.

1. Introduction

It is now becoming possible to fabricate systems in which electrons are confined within precisely controlled two-dimensional regions which are comparable in size to the de Broglie wavelength. Recent developments in this area are reviewed in a volume edited by Altshuler et al. [1]. In this paper we consider electrons confined in a quantum wire or electron waveguide. It is important to understand the effects of impurities in these systems, which increase the resistance of the wire and may lead to Anderson localisation. We present a theoretical analysis of the scattering of an electron propagating in a two-dimensional waveguide by a weak, localised impurity potential. We analyse resonances which occur when a normal mode crosses over from being evanescent to propagating as the energy of the electron is increased. We show that these resonances can either increase or decrease the probability of reflection of an electron by many orders of magnitude, depending on whether the electron energy is slightly above or below the resonant value.

These resonances have been noticed previously in calculations of the effect of impurities on the conductivity of quantum wires [2, 3], evaluated using a multi-channel version of the Landauer formula [4]. Surprisingly, in the case of an s-wave scatterer, it was discovered that all of the elements of the reflection matrix corresponding to propagating modes vanish simultaneously as the resonance is approached from below. This observation has been explained by Bagwell [2], using an argument which is specific to an s-wave or delta function scatterer. Chu and Sorbello [3] described a more general method for calculating the scattering matrix, which does not give explicit formulae simple enough for further analysis. In this paper we present a complementary approach to that of Bagwell, in that we give a perturbative theory for the transverse resonances, which is valid for a very general class of localised scattering potentials. Although the perturbation analysis is not straightforward, the formulae for the matrix elements have a very simple structure.

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For clarity we describe the effect in the simplest possible model. We consider the solution of the Schrödinger equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \frac{2\mu}{\hbar^2}[\varepsilon V(x, y) - E]\psi \tag{1.1}$$

in a channel in two dimensions: the wave function $\psi(x, y)$ satisfies the boundary conditions $\psi(x, 0) = \psi(x, L) = 0$. The potential $\varepsilon V(\boldsymbol{r})$ in the channel is close to zero, except in the neighbourhood of a scatterer near $x = 0$. The results can readily be extended to any waveguide of uniform cross-section in which none of the normal modes allows flux to escape from the sides (the latter restriction precludes applications to electromagnetic waves in optical fibres). Away from the scatterer, the solution of the Schrödinger equation can be expressed as a superposition of a finite set of forward and backward propagating normal modes, and an infinite set of evanescent modes, in which the wave function increases or decreases exponentially as a function of x. The amplitudes of the modes on either side of the scatterer are linearly related. Two types of matrix, the transfer matrix and the scattering matrix (which contains the reflection and transmission matrices as submatrices) can be used to express these linear relationships. These matrices and their interrelationships are described in Section 2.

When the scattering potential εV is small, the transfer matrices can be calculated perturbatively. The perturbation theory diverges when the resonance condition is met; in this two-dimensional case the resonance condition is that the channel width should be a half-integer multiple of the free-space de Broglie wavelength. In Section 3 we derive the form of the transfer matrices in the neighbourhood of the resonance, solving a truncated system of equations for the divergent terms exactly. The reflection and transmission matrices for a weak scatterer are computed from the transfer matrix in Section 4. We discuss the case of an s-wave scatterer in detail in Section 5, showing that at frequencies infinitesimally below the resonance there is no reflection from the scatterer.

2. Scattering Matrices and Transfer Matrices

In this section we discuss the definition of the transfer matrices and their relationship with the scattering matrix which we require. Although this relationship is well known [5], we have included this material because we have not found any discussion which provides a set of definitions and a notation which exactly matches our needs.

The solution of the Schrödinger equation can be written in the form of a superposition of normal modes $\phi_n^{\pm}$,

$$\begin{aligned}\psi(x, y) &= \sum_{n=1}^{\infty} [a_n(x) \exp(ik_n x) \sin(n\pi y/L) + b_n(x) \exp(-ik_n x) \sin(n\pi y/L)] \\ &= \sum_{n=1}^{\infty} [a_n(x)\, \phi_n^+(x, y) + b_n(x)\, \phi_n^-(x, y)]\,,\end{aligned} \tag{2.1}$$

where k_n is the wave vector for the n-th mode,

$$k_n = \left(\frac{2\mu E}{\hbar^2} - \frac{n^2\pi^2}{L^2}\right)^{1/2}. \tag{2.2}$$

If any of the k_n are zero, this expansion must be modified by replacing the sinusoidal x dependence of the wave function of the n-th mode with a linear function of x. The sum (2.1) includes both the propagating modes and the evanescent modes, for which k_n is imaginary: in these cases we take the root of (2.2) with positive imaginary part, so that the coefficients a_n multiply evanescent waves which decrease to the right (i.e. as x increases).

When the potential energy $\varepsilon V(x, y)$ is zero, the multipliers $a_n(x)$ and $b_n(x)$ are independent of x. If $V(x, y)$ vanishes sufficiently rapidly as $|x| \to \infty$, the effect of a localised scatterer can therefore be described by means of a linear transformation between the coefficients a_n^-, b_n^- far to the left of the scatterer and the coefficient a_n^+, b_n^+ far to its right. This linear relationship is described by a transfer matrix $\tilde{M}$, which can be decomposed into four submatrices as shown below,

$$\begin{pmatrix} \boldsymbol{a}^+ \\ \boldsymbol{b}^+ \end{pmatrix} = \tilde{M} \begin{pmatrix} \boldsymbol{a}^- \\ \boldsymbol{b}^- \end{pmatrix} = \begin{pmatrix} \tilde{M}_{oi} & \tilde{M}_{oo} \\ \tilde{M}_{ii} & \tilde{M}_{io} \end{pmatrix} \begin{pmatrix} \boldsymbol{a}^- \\ \boldsymbol{b}^- \end{pmatrix}. \tag{2.3}$$

The submatrices $\tilde{M}_{xx}$ and vectors $\boldsymbol{a}$, $\boldsymbol{b}$ are infinite-dimensional because there is an infinite number of evanescent modes. The subscript i and o on the submatrices of $\tilde{M}$ indicate whether the amplitudes being coupled by the submatrix represent ingoing waves, travelling toward the scatterer, or outgoing waves, moving away from it: for example, the submatrix $\tilde{M}_{oi}$ describes contributions to the amplitudes of the outgoing waves on the right, a_n^+, coming from the amplitudes a_n^- of the incoming waves to the left. Note that, with these conventions, we are defining the evanescent modes to be outgoing if they decay away from the scatterer, and incoming if they grow with increasing distance from the scatterer.

The transfer matrix is a useful mathematical tool for analysing the scatterer because the transfer matrices for successive scatterers combine multiplicatively. It is not of very much physical significance however, because it describes an experiment with unusual boundary conditions. The most physically significant description is in terms of the scattering matrix $\tilde{S}$, which consists of four submatrices describing transmission and reflection at the scatterer,

$$\begin{pmatrix} \boldsymbol{a}^+ \\ \boldsymbol{b}^- \end{pmatrix} = \tilde{S} \begin{pmatrix} \boldsymbol{a}^- \\ \boldsymbol{b}^+ \end{pmatrix} = \begin{pmatrix} \tilde{T}^+ & \tilde{R}^+ \\ \tilde{R}^- & \tilde{T}^- \end{pmatrix} \begin{pmatrix} \boldsymbol{a}^- \\ \boldsymbol{b}^+ \end{pmatrix}. \tag{2.4}$$

The element $R_{nm}^{\pm}$ therefore gives the amplitude for reflection from the m-th incoming mode on the right $(+)$ or left $(-)$ of the scatterer, into the n-th mode on the same side; the coefficients of the transmission matrices $\tilde{T}^{\pm}$ are interpreted similarly.

By comparing (2.3) and (2.4) we can express the reflection and transmission matrices in terms of the transfer matrices,

$$\begin{aligned} \tilde{T}^+ &= \tilde{M}_{oi} - \tilde{M}_{oo}\tilde{M}_{io}^{-1}\tilde{M}_{ii}, \qquad \tilde{T}^- = \tilde{M}_{io}^{-1}, \\ \tilde{R}^+ &= \tilde{M}_{oo}\tilde{M}_{io}^{-1}, \qquad \tilde{R}^- = -\tilde{M}_{io}^{-1}\tilde{M}_{ii}. \end{aligned} \tag{2.5}$$

When the scatterer is symmetric under reflection about $x = 0$, the two transmission and reflection matrices are identical, i.e. $\tilde{R}^+ = \tilde{R}^- = \tilde{R}$ and $\tilde{T}^+ = \tilde{T}^- = \tilde{T}$.

We end this section by giving an expression for the total probability of reflection for a particle initially in the m-th mode, this is

$$P_m = \sum_{n=1}^{N_R} \frac{k_n}{k_m} |R_{nm}|^2, \tag{2.6}$$

where N_p is the number of propagating modes in each direction. The factor k_n/k_m is required because the flux of particles in a given mode is proportional to the momentum $\hbar k_n$.

3. Perturbation Theory for the Transfer Matrix

By substitution into the Schrödinger equation we find the following equations of motion for the amplitudes $a_n(x)$, $b_n(x)$ defined by (2.1)

$$\frac{da_n}{dx} = \frac{\varepsilon\mu}{ik_n\hbar^2} \sum_{m=1}^{\infty} V_{nm}(x) \{\exp[i(k_m - k_n)x]\, a_m + \exp[-i(k_n + k_m)x]\, b_m\},$$

$$\frac{db_n}{dx} = \frac{-\varepsilon\mu}{ik_n\hbar^2} \sum_{m=1}^{\infty} V_{nm}(x) \{\exp[i(k_m + k_n)x]\, a_m + \exp[i(k_n - k_m)x]\, b_m\}, \tag{3.1}$$

where μ is the mass of the particle, and the $V_{nm}(x)$ are matrix elements of the potential $V(x, y)$, defined by

$$V_{nm}(x) = \frac{2}{L} \int_0^L dy \sin(n\pi y/L) \sin(m\pi y/L)\, V(x, y). \tag{3.2}$$

The matrix elements of the transfer matrices are obtained by propagating the solutions of these equations from $x = -\infty$ to $x = \infty$,

$$\begin{aligned}
(\tilde{M}_{oi})_{nm} &= \{a_n(+\infty) \mid a_{m'}(-\infty) = \delta_{mm'}, b_{m'}(-\infty) = 0, \forall m' \geqq 1\},\\
(\tilde{M}_{io})_{nm} &= \{b_n(+\infty) \mid b_{m'}(-\infty) = \delta_{mm'}, a_{m'}(-\infty) = 0, \forall m' \geqq 1\},\\
(\tilde{M}_{ii})_{nm} &= \{b_n(+\infty) \mid a_{m'}(-\infty) = \delta_{mm'}, b_{m'}(-\infty) = 0, \forall m' \geqq 1\},\\
(\tilde{M}_{oo})_{nm} &= \{a_n(+\infty) \mid b_{m'}(-\infty) = \delta_{mm'}, a_{m'}(-\infty) = 0, \forall m' \geqq 1\}.
\end{aligned} \tag{3.3}$$

We can solve the equations (3.1) for these coefficients pertubatively, by assuming that the coefficient which is non-zero at $x = -\infty$ remains equal to unity for all x, and that the other coefficients remain small enough that their contribution to the right-hand side of (3.1) can be neglected. This gives, to leading order in ε,

$$\begin{aligned}
(\tilde{M}_{oi})_{nm} &\sim \delta_{nm} + \frac{\varepsilon\mu}{ik_n\hbar^2} \int_{-\infty}^{\infty} dx\, e^{-i(k_m - k_n)x}\, V_{nm}(x) = \delta_{nm} + \frac{\varepsilon\mu}{ik_n\hbar^2} I_{nm}^{-*},\\
(\tilde{M}_{io})_{nm} &\sim \delta_{nm} - \frac{\varepsilon\mu}{ik_n\hbar^2} \int_{-\infty}^{\infty} dx\, e^{i(k_n - k_m)x}\, V_{nm}(x) = \delta_{nm} - \frac{\varepsilon\mu}{ik_n\hbar^2} I_{nm}^{-},\\
(\tilde{M}_{ii})_{nm} &\sim -\frac{\varepsilon\mu}{ik_n\hbar^2} \int_{-\infty}^{\infty} dx\, e^{i(k_n + k_m)x}\, V_{nm}(x) = \frac{\varepsilon\mu}{ik_n\hbar^2} I_{nm}^{+},\\
(\tilde{M}_{oo})_{nm} &\sim \frac{\varepsilon\mu}{ik_n\hbar^2} \int_{-\infty}^{\infty} dx\, e^{-i(k_m + k_n)x}\, V_{nm}(x) = \frac{\varepsilon\mu}{ik_n\hbar^2} I_{nm}^{+*}.
\end{aligned} \tag{3.4}$$

We will assume that the potential $V(x, y)$ is such that the integrals $I^{\pm}_{nm}$ defined by (3.4) converge, even for imaginary k_n, k_m. These perturbative solutions are expected to be valid provided

$$\frac{\varepsilon\mu W}{Lk_N\hbar^2} \ll 1\,, \tag{3.5}$$

where W is the integral of $V(x, y)$ over all space, and k_N is the wave vector with the smallest absolute value. The expressions (3.4) for the matrix elements $(\tilde{M}_{xx})_{nm}$ diverge as $|k_n| \to 0$: by varying the energy one of the k_n (the N-th, say) can be made arbitrarily small, as the mode crosses over between being propagating and evanescent. From (2.2) we see that this resonant condition occurs when the width of the channel is a half-integer multiple of the de Broglie wavelength. It is this resonant situation which is the principal subject of this paper, and we must therefore examine the solution of equations (3.1) for the case in which the simple perturbative solution described above is no longer justified for transfer into the N-th mode, which we will refer to as the critical mode.

We now consider the solution of (3.1) when both k_N and the perturbation ε are small. When ε is small, it is clear the variation of the coefficients a_n, b_n is small unless k_n is small. When considering the solutions with the boundary conditions (3.3), the only coefficients which are not small are therefore a_N, b_N, and the coefficients a_m or b_m which are unity at $x = -\infty$. We therefore consider the non-perturbative solution of the truncated system of equations in which only the terms in a_N, b_N, and one other coefficient a_m or b_m are retained. Unless $m = N$, we can set the 'driving' coefficient a_m or b_m equal to unity for all x. Having solved these truncated equations, we can use the solutions as a basis for the perturbative solution for the remaining coefficients.

We can only solve these truncated equations in the limit $k_n \to 0$, and the resulting expressions are only an accurate approximation to the exact solutions when $k_N\lambda \ll 1$, where λ is the range of x over which the scattering potential $V(x, y)$ is significantly different from zero. The range of applicability of this solution overlaps with that of the simple perturbation theory, specified by (3.5), provided

$$\frac{\varepsilon\mu W\lambda}{L\hbar^2} \ll 1\,. \tag{3.6}$$

We will assume that this condition is satisfied.

We must consider two separate cases of the truncated strongly coupled equations. First we consider the case where $b_N(-\infty) = 1$, which corresponds to finding the transfer matrix element $(\tilde{M}_{io})_{NN}$. In the limit $k_N \to 0$, the truncated equations for the a_N and b_N are

$$\frac{\mathrm{d}a_N}{\mathrm{d}x} = \frac{\varepsilon\mu}{ik_N\hbar^2} V_{NN}(x)\,[a_N(x) + b_N(x)] = -\frac{\mathrm{d}b_N}{\mathrm{d}x}\,, \tag{3.7}$$

which must be solved with the boundary conditions $a_N(-\infty) = 0$, $b_N(-\infty) = 1$. The solutions of the truncated equations are

$$(\tilde{M}_{io})_{NN} \sim b_N(\infty) = 1 - a_N(\infty) = 1 - \frac{\varepsilon\mu}{ik_N\hbar^2}\int_{-\infty}^{\infty} \mathrm{d}x\, V_{NN}(x)\,. \tag{3.8}$$

Secondly, we must consider the case where $b_m(-\infty) = 1$, with $m \neq N$, which corresponds to finding the transfer matrix element $(\tilde{M}_{io})_{Nm}$. In this case the truncated equations are, in the limit $k_N \to 0$,

$$\frac{da_N}{dx} = \frac{\varepsilon\mu}{ik_N\hbar^2}\{V_{NN}(x)[a_N(x) + b_N(x)] + V_{Nm}(x)\,e^{-ik_m x}\,b_m(x)\} = -\frac{db_N}{dx}, \tag{3.9}$$

which must be solved with the boundary conditions $a_N(-\infty) = b_N(-\infty) = 0$. The solutions of (3.9) are

$$(\tilde{M}_{io})_{Nm} \sim b_N(\infty) = -a_N(\infty) = -\frac{\varepsilon\mu}{ik_N\hbar^2}\int_{-\infty}^{\infty} dx\, V_{Nm}(x)\,e^{-ik_m x}. \tag{3.10}$$

We have found that, surprisingly, the expressions (3.8) and (3.10) for the strongly coupled matrix elements are exactly the same as for those given by the $k_N \to 0$ limit of perturbation theory, (3.4). We emphasise that (3.8) and (3.10) remain valid even when these matrix elements are large, provided (3.6) is satisfied.

The perturbative solutions for all the matrix elements $(\tilde{M}_{xx})_{nm}$ with $n, m \neq N$ remain unchanged, and are still given by (3.4) in the neighbourhood of the resonance. The matrix elements $(\tilde{M}_{xx})_{nN}$ are modified by the resonance, because the driving term a_N or b_N is now a function of x, given by solving (3.7), rather than unity. These elements can also be calculated in the region of the resonance by perturbation theory, but we do not present the results because they are not required for our subsequent analysis.

We end this section by commenting that, if the scattering potential is so strongly localised that it is negligible at the edges of the channel, the integral I_{nm} can be expressed in terms of the Fourier transform of the scattering potential $V(x, y)$. The elements of the transfer matrix, given by (3.4), can therefore be related to the Born formula [6] for the scattering cross-section in free space.

4. Transverse Resonances

In Section 3 we obtained a theory for the transfer matrix in the limit of a weak potential $V(x, y)$. At a typical energy, simple perturbation theory is adequate. At 'resonant' energies, where the wave number k_N of the critical mode is small, we must use a non-perturbative solution for the transfer matrix elements $(\tilde{M}_{xx})_{Nm}$. In this section we compute the reflection matrix $\tilde{R}^+$ using (2.5) and the approximate transfer matrices derived in Section 3. The other submatrices of the scattering matrix can be calculated by the same method.

In order to calculate $\tilde{R}^+$ we must find an analytic approximation to $\tilde{M}_{io}^{-1}$. The matrix $\tilde{M}_{io}$ can be decomposed into the sum of the identity matrix, a matrix $\tilde{X}$ which only has non-zero elements in the N-th row, and a remainder $\tilde{m}_{io}$ which has vanishing elements in the N-th row,

$$\tilde{M}_{io} = \tilde{I} + \tilde{X} + \tilde{m}_{io},$$

$$(\tilde{M}_{io})_{nm} = \delta_{nm} + \delta_{Nn}X_m + (\tilde{m}_{io})_{nm}, \qquad (\tilde{m}_{io})_{Nm} = 0. \tag{4.1}$$

The coefficients of $\tilde{m}_{io}$ are always small when ε is small, but the coefficients of $\tilde{X}$ can be very large if the energy is close to resonance. We can obtain the inverse of $\tilde{M}_{io}$ by computing

the inverse of $\tilde{I} + \tilde{X}$ exactly, and then treating the remainder $\tilde{m}_{io}$ as a small perturbation. By inspection, the elements of the inverse of $\tilde{I} + \tilde{X}$ are

$$(\tilde{I} + \tilde{X})^{-1}_{nm} = \delta_{nm} - \delta_{nN} \frac{X_m}{1 + X_N}. \tag{4.2}$$

We can now compute our approximate expression for the reflection matrix,

$$\begin{aligned} \tilde{R}^+ &= \tilde{M}_{oo}(\tilde{I} + \tilde{X} + \tilde{m}_{io})^{-1} \\ &\sim \tilde{M}_{oo}(\tilde{I} + \tilde{X})^{-1}(\tilde{I} + \tilde{X} - \tilde{m}_{io})(\tilde{I} + \tilde{X})^{-1}. \end{aligned} \tag{4.3}$$

Using (4.2), and dropping those terms which make $O(\varepsilon^2)$ contributions, we find the following expression for the elements of $\tilde{R}^+$:

$$R^+_{nm} \sim (\tilde{M}_{oo})_{nm} - (\tilde{M}_{oo})_{nN} \frac{X_m}{1 + X_N}. \tag{4.4}$$

By inspection of (4.1), we find that $X_m = (\tilde{M}_{io})_{Nm} - \delta_{Nm}$, and (4.4) can be expressed in terms of elements of the transfer matrices as follows:

$$R^+_{nm} = (\tilde{M}_{oo})_{nm} - \frac{(\tilde{M}_{oo})_{nN}(\tilde{M}_{io})_{Nm}}{(\tilde{M}_{io})_{NN}} + O(\varepsilon^2). \tag{4.5}$$

This is our principal result for the elements of the reflection matrix. Very similar expressions can be obtained for other elements of the scattering matrix using essentially the same method, for example,

$$T^-_{nm} = (\tilde{M}_{io})_{nm} - \frac{(\tilde{M}_{io})_{nN}(\tilde{M}_{io})_{Nm}}{(\tilde{M}_{io})_{NN}} + O(\varepsilon^2). \tag{4.6}$$

In the remainder of this paper we consider the implications of these expressions ((4.5) and (4.6)), using the formulae (3.4), (3.8), and (3.10) for the matrix elements.

Away from the resonance, the second term in (4.5) or (4.6) is negligible, because both terms in the numerator are $O(\varepsilon)$, and the denominator is close to unity. In the neighbourhood of the resonance, when k_N is small, the constant term in (3.8) can be neglected. In the limit $k_N \to 0$ the matrix element R^+_{nm} is therefore

$$\lim_{k_N \to 0} R^+_{nm} \sim R^{+(0)}_{nm} \left[1 - \frac{I^+_{nN} * I^-_{Nm}}{I^-_{NN} * I^+_{nm}} \right], \tag{4.7}$$

where $R^{+(0)}_{nm} = (\tilde{M}_{oo})_{nm}$ is the value of the matrix element away from resonance, and the $I^{\pm}_{nm}$ are defined in (3.4). It is clear from this expression that the resonance can have a strong effect on the reflection probabilities.

We wrote a computer program to investigate the resonances. Fig. 1 shows numerically computed reflection intensities for a non s-wave scatterer, plotted as a function of energy in the neighbourhood of a resonance. The parameters of the model were $L = \pi$, $\mu = 1$, $\hbar = 0.25$, and the potential was a Gaussian, $v(R) = \exp(-R^2/2R_0^2)$, where R is the distance from the centre of the scatterer at (x_0, y_0); we used the parameters $R_0 = 0.2$, $\varepsilon = 0.005$, $x_0 = 0$ and $y_0 = 0.55L$. The numerically computed values of $|R_{55}|^2$ are in excellent agreement with those calculated from equation (4.5).

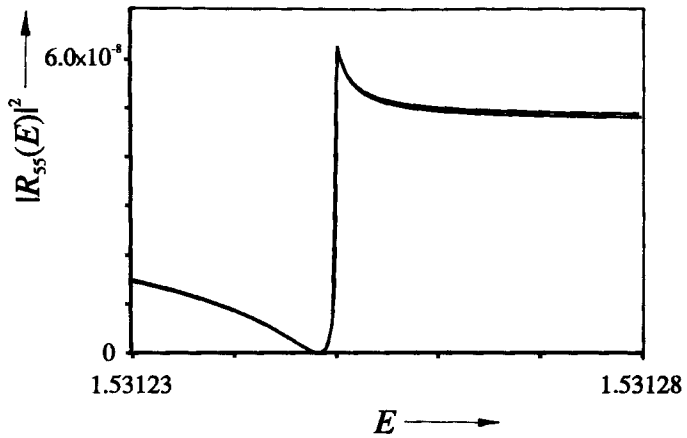

Fig. 1. Numerically computed reflection intensity $|R_{55}(E)|^2$ for a non s-wave scatterer, close to the $N = 7$ channel resonance, compared with equation (4.5). Where they differ, the lower lying curve is the perturbation theory result

5. The Case of s-Wave Scattering

Now we consider the case of an s-wave scatterer in some detail. In this case the scattering potential decays to zero over a distance which is small compared to the de Broglie wavelength, and the integrals $I^{\pm}_{nm}$ are proportional to the product of the normal mode wave functions $\phi_n^+(x, y)$ and $\phi_n^-(x, y)$ (defined in (2.1)) evaluated at the position of the scatterer, $y = y_0$. We therefore have

$$I^{\pm}_{nm} \sim \frac{2W}{L} \sin(n\pi y_0/L) \sin(m\pi y_0/L), \tag{5.1}$$

where W is the integral of $V(\boldsymbol{r})$ over all space. When the $I^{\pm}_{nm}$ are given by (5.1), it is clear that the reflection coefficient at resonance (4.7) vanishes, because each of the $I^{\pm}_{nm}$ is the product of two terms which are functions of n and m only. The value of the reflection coefficient therefore approaches zero at resonance, to within the $O(\varepsilon^2)$ error of the approximation scheme used.

The form of the reflection coefficient close to the resonance is universal in the case of s-wave scattering: from (4.5) and (5.1) we find the following expression for the dependence of the reflection amplitude on k_N:

$$R_{nm} = R^{(0)}_{nm}\left[\frac{k_N}{k_N + i\varkappa}\right] + O(\varepsilon^2), \tag{5.2}$$

where

$$\varkappa = \frac{2\varepsilon\mu W}{\hbar^2 L} \sin^2(N\pi y_0/L). \tag{5.3}$$

(This result was previously obtained by Bagwell [2].) The asymmetric lineshape (5.2) is plotted in Fig. 2a; E_0 is the energy at which $k_n = 0$, and the width parameters is $\Delta E = \varkappa^2\hbar^2/2\mu$.

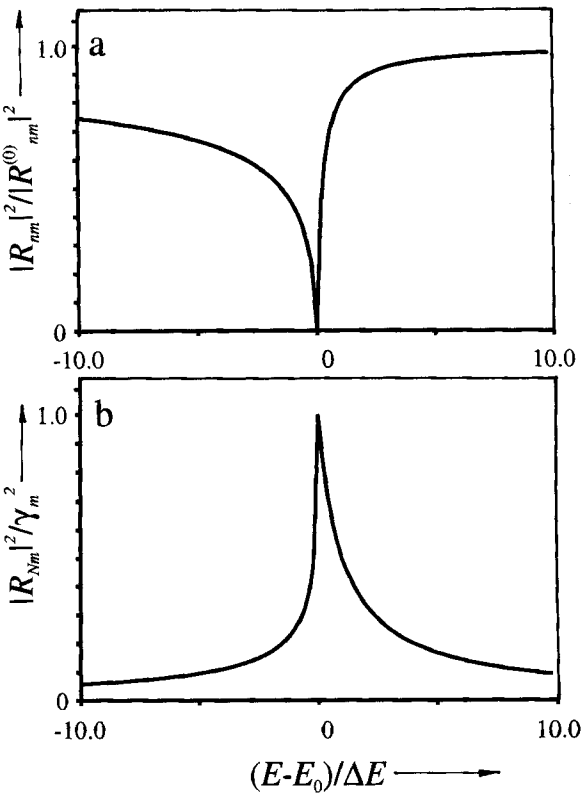

Fig. 2. Theoretical lineshapes of the resonance as a function of energy for s-wave scatterer a) $|R_{nm}(E)|^2$, given by (5.2), b) $|R_{Nm}(E)|^2$, given by (5.5)

Equation (5.2) characterises the form of the reflection matrix elements R_{nm} when $n, m < N$ (i.e. when both the n-th and the m-th modes are non-critical propagating modes). The reflection coefficient R_{Nm} for reflection into the critical mode from a propagating mode $m < N$ behaves somewhat differently. It can be calculated by exactly the same method, starting from (4.5) and setting $n = N$. The matrix elements $(\tilde{M}_{oo})_{Nm}$ and $(\tilde{M}_{oo})_{NN}$ can be calculated using the same methods as for (3.8) and (3.10),

$$(\tilde{M}_{oo})_{Nm} \sim \frac{2\varepsilon\mu W}{ik_N\hbar^2} \sin\left(\frac{m\pi y_0}{L}\right) \sin\left(\frac{N\pi y_0}{L}\right),$$

$$(\tilde{M}_{oo})_{NN} \sim \frac{2\varepsilon\mu W}{ik_N\hbar^2} \sin^2\left(\frac{N\pi y_0}{L}\right) \tag{5.4}$$

in the limit $k_N \to 0$. Hence we find

$$R_{Nm} \sim \frac{\gamma_m \varkappa}{ik_n - \varkappa}, \qquad \gamma_m = \frac{\sin(m\pi y_0/L)}{\sin(N\pi y_0/L)}. \tag{5.5}$$

This lineshape is plotted in Fig. 2b.

We now summarise the results with a discussion of the properties of the reflection matrix close to resonance. The behaviour is very different, depending on the side from which the

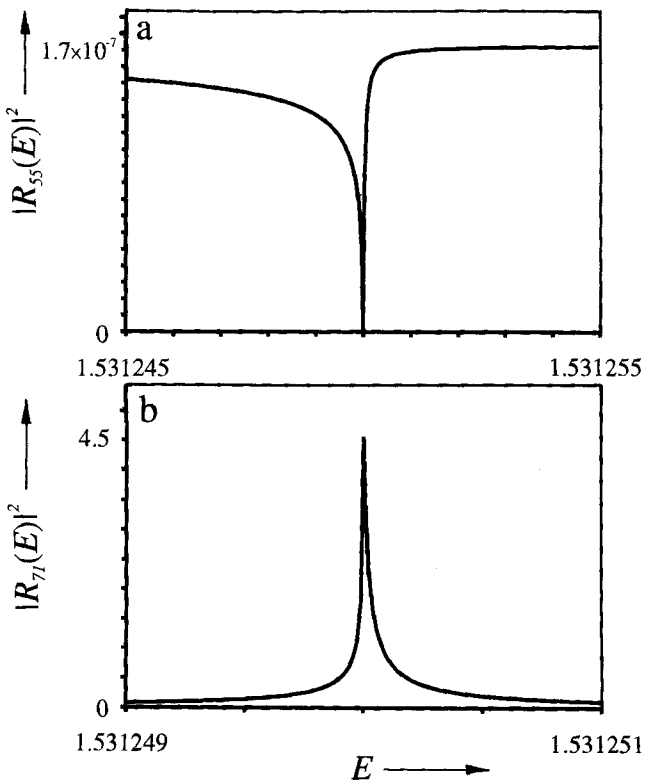

Fig. 3. Numerically computed reflection intensities for an s-wave scatterer, close to the $N = 7$ channel resonance a) $|R_{55}(E)|^2$, b) $|R_{71}(E)|^2$

resonance is approached. Slightly above the resonant energy, the wave vector of the critical mode is real. As the resonance is approached, the amplitudes R_{nm} for reflection into all of the propagating modes except the critical one decrease according to (5.2). The amplitude R_{Nm} for reflection into the critical mode increases according to (5.5). The probability of reflection P_m is therefore dominated by the reflection into the N-th mode, and is given by

$$P_m \sim \frac{k_N}{k_m} \frac{\gamma_m^2 \varkappa^2}{\varkappa^2 + k_N^2}, \tag{5.6}$$

which has a maximum value

$$P_m^{\max} = \frac{\gamma_m^2 \varkappa}{2k_m} = \frac{\varepsilon \mu W}{k_m \hbar^2 L} \sin^2\left(\frac{m\pi y_0}{L}\right). \tag{5.7}$$

This is much larger than the non-resonant reflection probability, which is $O(\varepsilon^2)$. On the low-energy side of the resonance, where the critical mode has a small imaginary wave vector, the critical mode makes no contribution to the probability of reflection (2.6). On this side of the resonance, the amplitudes for reflection into all of the propagating modes vanish as the resonance is approached: surprisingly, the scatterer is rendered invisible by the presence of the two mirrors (i.e. the two sides of the channel) on either side of it.

We verified these predictions using our computer program, with $R_0 = 0.008$, $\varepsilon = 1$, and the other parameters left unchanged. These parameters give a resonance in the $N = 7$ mode at energy $E_0 = 1.53125$ exactly. The numerical results are shown in Fig. 3: they are almost indistinguishable from the theoretical curves given by (5.2), with the width parameter $\Delta E = \varkappa^2\hbar^2/2\mu = 2.2 \times 10^{-8}$ obtained from (5.3).

6. Concluding Remarks

We have shown that, for the case of an s-wave scatterer, the total reflection probability is $O(\varepsilon^4)$ at an energy infinitesimally below the resonant energy (equation (5.2)), and $O(\varepsilon)$ just above the resonance (equation (5.7)). For an energy not close to resonance the reflection probability is $O(\varepsilon^2)$, in agreement with what would be expected from the Born formula. The reflection probability can therefore be either much less than or much greater than the non-resonant value, depending on whether the energy is just above or just below the resonance.

Our results were derived for the simplest possible model, a two-dimensional channel with hard walls, but the reader may readily verify that they generalise to three-dimensional problems and to systems in which the unperturbed potential is any function $V_0(y)$ with a minimum confining particles in the channel.

A simple way to observe the resonances may be to examine a disordered system containing a large number of randomly positioned s-wave scatterers. The small reflections from each individual scatterer result in an exponential decay of the transmission matrix as a function of length, and in the occurrence of localised eigenfunctions [5]. At energies slightly above the resonance the localisation length would be decreased due to the enhanced backscattering. It may also be possible to observe the vanishing of the reflection matrix below the resonance frequency as a divergence of the localisation length, but there is, however, a significant complication here. The successive scatterers can only be regarded as independent if the amplitude reflected into the evanescent critical mode is able to decay to negligible proportions before reaching adjacent scatterers. This requires that the distance between scatterers be very large compared to the decay length $1/k_N$, but (5.2) implies that to observe the resonance we require $k_N < \varkappa$, and $\varkappa$ is itself a small quantity. It is therefore clear that the scatterers would have to be widely spaced in order to be regarded as independent; we will not give a detailed estimate.

Concerning other possible applications of the results, it is clear that with a suitable change of notation they apply to any problem involving a waveguide with perfectly reflecting walls: this would include models for microwave guides, and sound and water waves in channels as well as the quantum mechanical model we have discussed. The analysis does assume, however, that there exists a normalisable eigenfunction $\phi_N(x, y)$ corresponding to the resonant mode ($k_N \approx 0$). This precludes any applications to optical fibres, where the radiation is able to escape from the fibre for low values of k_n (which correspond to the wave vector being at a large angle to the axis of the fibre) [7].

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