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A Quantum Mechanical Treatment of the Mirror Electron Microscope

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SUMMARY

A wave mechanical description of the electron beam in a mirror electron microscope is given. First the Schrödinger equation of the electron beam is set up, from which the wave function is obtained. Then the probability current density is derived, which turns out to be a useful expression to clarify the formation of the image on the screen.

INTRODUCTION

This article contains a wave mechanical description of the electron beam in a mirror electron microscope. The tackling procedure is first to set up the Schrödinger equation of the electron beam, then to look for the wave function that satisfies it, and afterwards to derive the probability current density which turns out to be a useful expression to clarify the formation of the image on the screen. Applying this procedure at first to the case of a microscope without specimen, the unperturbed path of the electrons is found.

When the influence of the specimen, expressed by a small perturbation term in Schrödinger's equation, is taken into account, the approach becomes much more difficult. Application of a perturbation method, which is more or less obvious in this case, does not lead to an entirely satisfactory solution; by means of the W.K.B. method and Langer's method together, the problem can be solved in a better way. Finally the validity of the solutions obtained is discussed in appendix A.

Airy functions which are used freely in this article, are dealt with briefly in appendix B.

1. Principle of the Mirror Electron Microscope

Contrary to most of the other electron microscopes, the mirror electron microscope, [2], has a reflecting electron beam. It arrives monoenergetically and parallel at the retarding field of an electrostatic mirror, is slowed down, and then reverses. The specimen surface, which is chosen to be the negative mirror electrode, has been given a slightly more negative electric potential then the energy of the incident beam, which causes the electrons to reverse very near the specimen surface, but without actually touching it. Consequently the surface is protected against damage as a result of electron bombardment. (See fig. 1)

Near the plane of reversal, the electron beam is highly sensitive to perturbations disturbing the flatness of the reflecting equipotential plane. These perturbations may be caused by electrostatic or topographic irregularities on the specimen surface, because this is positioned at a very short distance from the plane of reflection. So the reversing beam carries information concerning the specimen surface in the form of a small perturbation. The information can be made visible by projecting the beam onto a screen, whereas the contrast of the image can be provided by placing an aperture in the reversing beam.

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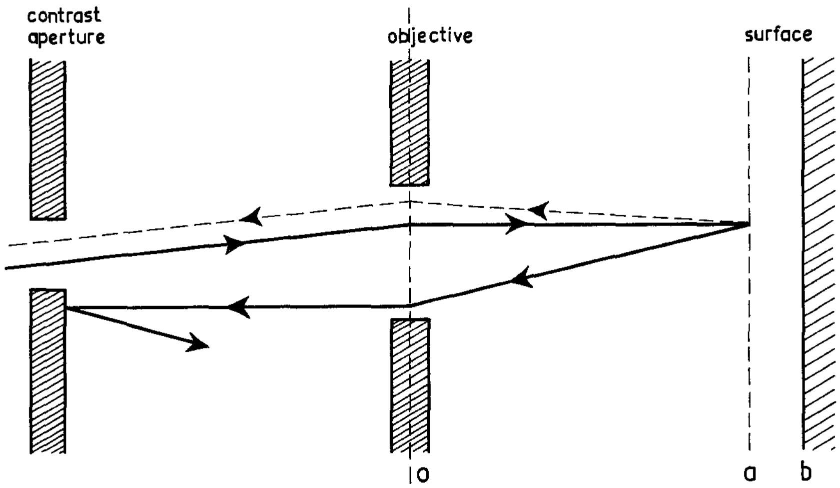

Figure 1. Electron trajectories in the mirror electron microscope.

2. The Microscope without Specimen

The unperturbed model consists of a parallel beam of electrons of kinetic energy E, running in the direction of positive x, being slowed down by a homogeneous electrostatic retarding field. Reflection takes place in the plane $x=a$, whereas the specimen surface is located at $x=b$. All electrons travel to and fro along the same axial trajectories, so that the problem is considered to be one-dimensional. In our configuration, four regions are distinguished: (see fig. 2)

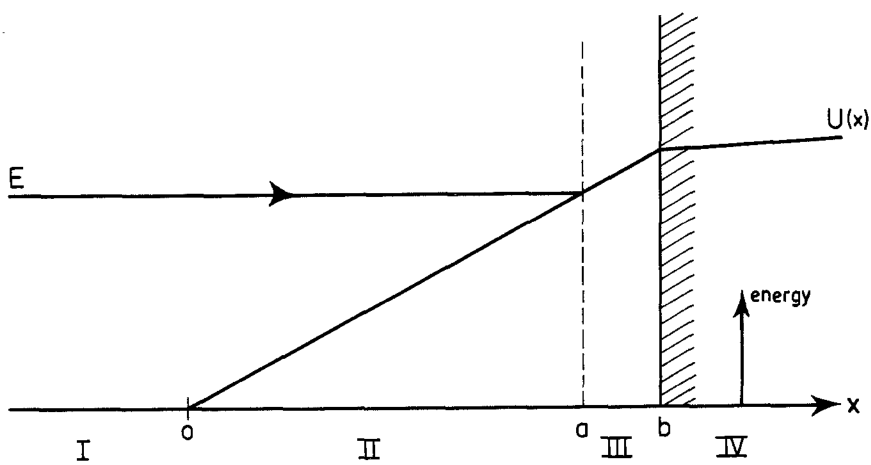

Figure 2. Potential energy in the different regions.

region I: electron beam of constant energy E $(x<0)$
region II: retarding field before point of reversal $(0<x<a)$
region III: retarding field beyond point of reversal $(a<x<b)$
region IV: specimen $(x>b)$

In all regions the electron beam may be characterised by the wave function ψ, satisfying Schrödinger's time independent equation for one electron, [5], [6]:

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\{E-U(x)\}\psi=0\,.$$

where m=electron rest mass,

$\hbar = h/2\pi$, h = Planck constant,
$U(x)$ = potential energy of retarding field.

In region I, where $U(x)=0$, we find immediately

$$\psi^{\mathrm{I}} = C_1 \exp(i\sigma x) + C_2 \exp(-i\sigma x)\,,$$

$\sigma = (2mE)^{\frac{1}{2}}/\hbar$ meaning the wave number of the electron waves.

In the regions II and III, the potential energy in the homogeneous retarding field is a function, linear in x, and equalling the original kinetic energy E in the point of reversal $x=a$

$$U(x) = \frac{E}{a}\,x\,,$$

so that the Schrödinger equation becomes

$$\frac{d^2\psi^{\mathrm{II,III}}}{dx^2} + \sigma^2\left(\frac{a-x}{a}\right)\psi^{\mathrm{II,III}} = 0\,.$$

Substitution of

$$\xi = (\sigma a)^{\frac{2}{3}}\left(\frac{x-a}{a}\right)$$

leads to the differential equation

$$\frac{d^2\psi^{\mathrm{II,III}}}{d\xi^2} - \xi\psi^{\mathrm{II,III}} = 0\,,$$

known under the name of Airy equation, whose solutions $Ai(\xi)$ and $Bi(\xi)$ are called Airy functions of the first and second kind (see appendix). Both of them show an oscillatory behaviour for $\xi<0$ (region II), but for $\xi>0$ (region III) $Ai(\xi)$ decreases while $Bi(\xi)$ increases exponentially. Taking the physical circumstances into account, we must conclude therefore that $Bi(\xi)$ cannot be used here, and that

$$\psi^{\mathrm{II,III}} = C_3\,Ai(\xi) \tag{1}$$

is the complete solution in region II and III. For large negative values of ξ, this may be approximated by the asymptotic representation

$$\psi^{\mathrm{II}} = \frac{C_3}{\pi^{\frac{1}{2}}}\,|\xi|^{-\frac{1}{4}}\cos\left(\tfrac{2}{3}|\xi|^{\frac{3}{2}} - \frac{\pi}{4}\right)$$

or, after having separated incident and returning wave,

$$\psi^{\mathrm{II}} = \frac{C_3}{2\pi^{\frac{1}{2}}}\,|\xi|^{-\frac{1}{4}}\left\{\exp\left(\tfrac{2}{3}i|\xi|^{\frac{3}{2}} - \frac{\pi i}{4}\right) + \exp\left(-\tfrac{2}{3}i|\xi|^{\frac{3}{2}} + \frac{\pi i}{4}\right)\right\}.$$

Replacing x for ξ, we obtain the incident wave

$$\psi^{\mathrm{II}}_{+} = \frac{C_3}{2\pi^{\frac{1}{2}}}\,(\sigma a)^{-\frac{1}{6}}\left(\frac{a}{a-x}\right)^{\frac{1}{4}}\exp\left\{-\tfrac{2}{3}i\sigma a\left(\frac{a-x}{a}\right)^{\frac{3}{2}} + \frac{\pi i}{4}\right\} \tag{2}$$

and the returning wave

$$\psi^{\mathrm{II}}_{-} = \frac{C_3}{2\pi^{\frac{1}{2}}}\,(\sigma a)^{-\frac{1}{6}}\left(\frac{a}{a-x}\right)^{\frac{1}{4}}\exp\left\{\tfrac{2}{3}i\sigma a\left(\frac{a-x}{a}\right)^{\frac{3}{2}} - \frac{\pi i}{4}\right\}. \tag{3}$$

The constant C_3 can be expressed in C_1, by requiring ψ to be continuous while crossing from region I to II. In $x=0$ holds

$$\psi^{\mathrm{I}}_{+} = C_1$$

$$\psi^{\mathrm{II}}_{+} = \frac{C_3}{2\pi^{\frac{1}{2}}}\,(\sigma a)^{-\frac{1}{6}}\exp\left(-\tfrac{2}{3}i\sigma a + \frac{\pi i}{4}\right),$$

so that

$$C_3 = C_1\, 2\pi^{\frac{1}{2}}(\sigma a)^{\frac{1}{6}} \exp\left(\tfrac{2}{3}i\sigma a - \frac{\pi i}{4}\right) \tag{4}$$

fulfills the boundary requirements, changes (2) into

$$\psi^{\mathrm{II}}_{+} = C_1\left(\frac{a}{a-x}\right)^{\frac{1}{4}} \exp\left[-\tfrac{2}{3}i\sigma a\left\{\left(\frac{a-x}{a}\right)^{\frac{3}{2}} - 1\right\}\right], \tag{5}$$

and (3) into

$$\psi^{\mathrm{II}}_{-} = C_1\left(\frac{a}{a-x}\right)^{\frac{1}{4}} \exp\left[\tfrac{2}{3}i\sigma a\left\{\left(\frac{a-x}{a}\right)^{\frac{3}{2}} + 1\right\}\right]\cdot \exp\left(-\frac{\pi i}{2}\right). \tag{6}$$

In a similar way the returning beams in region I and II are connected. Here the boundary condition

$$C_2 = C_1 \exp\left(\tfrac{4}{3}i\sigma a - \frac{\pi i}{2}\right)$$

yields

$$\psi^{\mathrm{I}} = C_1 \exp(i\sigma x) + C_1 \exp\{-i\sigma(x - \tfrac{4}{3}a)\} \exp\left(-\frac{\pi i}{2}\right)$$

as a final expression for region I.

The wave functions (5) and (6) hold for large negative values of ξ, and since

$$\xi = \left\{\frac{(2mE)^{\frac{1}{2}}}{\hbar}\, a\right\}^{\frac{2}{3}} (x-a),$$

we may conclude that they lose validity at an extremely small distance from the reversal point, i.e. for $a-x$ sufficiently small. In this small region another expansion of $Ai(\xi)$ may be applied, namely its Taylor series for small values of the argument. However this does not provide very important results, so that we confine ourselves to giving the first term of the series

$$\psi(0) = C_3\, Ai(0) = C_3 \frac{3^{-\frac{2}{3}}}{\Gamma(\frac{2}{3})}$$

referring to the appendix for higher order terms.

In region III, beyond the small region where Taylor's series can be used, an expansion for large positive values of ξ is applicable to the Airy function. Using the same expression (4) for C_3, we find thus

$$\psi^{\mathrm{III}} = C_1\left(\frac{a}{x-a}\right)^{\frac{1}{4}} \exp\left\{-\tfrac{2}{3}\sigma a\left(\frac{x-a}{a}\right)^{\frac{3}{2}}\right\} \exp\left(\tfrac{2}{3}i\sigma a - \frac{\pi i}{4}\right)$$

which decreases rapidly away from the reversal point, because σ is very large.

The same exponentially decreasing behaviour is observed in region IV, and therefore it is not of much interest here.

3. The Microscope with Specimen

Up to now we examined only the microscope itself and the relatively simple wave function of its unperturbed electron field. If we place a specimen in it now, putting its surface in the transversal plane $x=b$, the small irregularities with regard to flatness or electrical charge distribution of the surface will bring about a perturbation in the electron field. This perturbation casuses tangential impulses to the electrons, which makes the problem three dimensional. However we consider only an axial plane, containing an x coordinate in the running direction of the electrons, and an y coordinate in tangential direction. Extension to the third dimension would not make the problem essentially different, only more confusing.

Our purpose in this chapter is to find the wave functions in the perturbed electron field.

1. Schrödinger's Equation in the Perturbed Field

The 2-dimensional time independent Schrödinger equation, [5], [6]:

$$\Delta\psi + \frac{2m}{\hbar^2}\{E - U(x, y)\}\psi = 0 \tag{7}$$

contains the potential energy term $U(x, y)$, now including a perturbation. Decomposing this term into the Fourier series

$$U(x, y) = U_0(x) + U_1(x)\cos ky + U_2(x)\cos 2ky + U_3(x)\cos 3ky + \dots,$$

we can identify $U_0(x)$ at once with the retarding potential, having the following values in the different regions:

$$U_0^{\mathrm{I}}(x) = 0$$

$$U_0^{\mathrm{II,III}}(x) = \frac{E}{a}x$$

$$U_0^{\mathrm{IV}}(x) = E\frac{b}{a}.$$

The sum of the Fourier series has to satisfy the Laplace field equation, and all the separated terms of it must do so as well, since the equation is homogeneous. $U_0(x)$ clearly satisfies it; $U_1(x)$ only if

$$\Delta U_1(x)\cos ky = 0, \text{ or}$$

$$\frac{d^2U_1(x)}{dx^2} - k^2U_1(x) = 0$$

which leads to

$$U_1(x) = c\,e^{kx}$$

(solution $c\,e^{-kx}$ is not in accordance with the physical requirement for $U_1(x)$ to decrease for decreasing x). The point $x=b$, $y=0$ on the specimen surface, where we assume the perturbation amplitude of the first order harmonic to be B_1, enables us to find the constant c from

$$c\,e^{kb} = B_1.$$

So the second term of the Fourier series yields

$$B_1 e^{k(x-b)}\cos ky.$$

Similarly the n^{th} term is found to be

$$B_n e^{nk(x-b)}\cos nky. \tag{8}$$

We must assume now that $\Sigma_{n=1}^{\infty}|B_n| \ll E$ in order to keep the perturbation energy small in comparison with the kinetic energy of the incident beam.

Insertion of (8) into the Schrödinger equation (7) gives

$$\Delta\psi + \frac{2m}{\hbar^2}[E - U_0(x) - B_1 e^{k(x-b)}\cos ky - B_2 e^{2k(x-b)}\cos 2ky - \dots]\psi = 0,$$

or more briefly

$$\Delta\psi+\sigma^2 M(x, y)\psi=0\ ; \tag{9}$$

with

$$M(x, y)=1-\frac{U_0(x)}{E}-\frac{B_1}{E}\,e^{k(x-b)}\cos ky-\frac{B_2}{E}\,e^{2k(x-b)}\cos 2ky-\ldots$$

Herewith we have reached the equation which will hold our attention.

2. Expansion with respect to the large parameter σ.
We assume

$$\left|\frac{\partial^2\psi}{\partial y^2}\right| \gg \left|\frac{\partial^2\psi}{\partial x^2}\right|, \text{ (see appendix A)}$$

making Schrödinger's equation dependent only on x as variable, and disrating y to parameter:

$$\frac{d^2\psi}{dx^2}+\sigma^2 M(x, y)\psi=0\,. \tag{10}$$

Here we need not identify $M(x, y)$ precisely, because we consider it to be a general function in x and y.

An approximate solution of (10) is obtained by applying the so-called W.K.B. method, starting from the separation of modulus and phase of the wave function

$$\psi=A\exp(i\sigma S)\,.$$

Substitution in (10) gives

$$\sigma^2 S_x^2-i\sigma\left(S_{xx}+2\frac{A_x}{A}S_x\right)-\frac{A_{xx}}{A}=\sigma^2 M(x, y)\,. \tag{11}$$

If we take only factors of σ^2 into account at first, (11) reduces to

$$S_x^2=M(x, y)$$

resulting in

$$S=\pm\int^x\sqrt{M(t, y)}\,dt\,,$$

with one integral boundary, necessary in order to be able to fulfil boundary conditions, still undefined; the $\pm$ sign refers to the difference between incident and returning beam.

Furthermore, the factor of σ in (11) yields

$$S_{xx}+2\frac{A_x}{A}S_x=0$$

leading to

$$A=S_x^{-\frac{1}{2}}=c\,M^{-\frac{1}{4}}(x, y)\,.$$

Herewith we know modulus and phase of the wave function up to second order terms, so that we are able to essemble the complete function

$$\psi=\frac{c}{M^{\frac{1}{4}}(x, y)}\exp\left(i\sigma\int^x\sqrt{M(t, y)}\,dt\right)+\frac{c}{M^{\frac{1}{4}}(x, y)}\exp\left(-i\sigma\int^x\sqrt{M(t, y)}\,dt\right).$$

The constant c and the undefined integral boundaries are now required to fulfil certain conditions. First of all the incident beam must satisfy

$$\psi_+=C_1 \text{ at } x=0$$

from which we derive

$$\psi_+=\frac{C_1}{M^{\frac{1}{4}}(x, y)}\exp\left(i\sigma\int_0^x\sqrt{M(t, y)}\,dt\right). \tag{12}$$

Then the connection between incident and returning beam at $x=a$, requires

$$\operatorname{mod}\ \{\psi_+(a)\} = \operatorname{mod}\ \{\psi_-(a)\}$$
$$\operatorname{phase}\{\psi_+(a)\} = \operatorname{phase}\{\psi_-(a)\} + \pi/2$$

with a phase-shift in the point of reversal, in order to connect with the unperturbed solutions. The conditions are both satisfied by

$$\psi_- = \frac{C_1}{M^{\frac{1}{4}}(x, y)} \exp\left(i\sigma \int_0^a \sqrt{M(t, y)}\mathrm{d}t - i\sigma \int_a^x \sqrt{M(t, y)}\mathrm{d}t\right) \exp\left(-\frac{\pi i}{2}\right). \tag{13}$$

However, (12) and (13) are not satisfactory in the neighbourhood of the reversal point where $M=0$, because the modulus of ψ is unbounded there. Therefore we shall look for a solution of (10) remaining bounded at $x=a$, and overlapping and agreeing with (12) and (13) away from the reversal point.

Let

$$\psi^{\mathrm{II}} = g(x) \cdot w(\zeta)$$

and ζ a function of x

$$\zeta = \zeta(x).$$

Substituting this in Schrödinger's equation (10)

$$g\zeta'^2 \frac{d^2 w}{d\zeta^2} + (2g'\zeta' + g\zeta'') \frac{dw}{d\zeta} + (g'' + g\sigma^2 M(x, y))w = 0 \tag{14}$$

($'$ means derivation to x)
and equating the factor of $dw/d\zeta$ to zero

$$2g'\zeta' + g\zeta'' = 0,$$

we deduce the expression

$$g(x) = c(\zeta')^{-\frac{1}{2}} \tag{15}$$

which converts (14) into

$$\frac{d^2 w}{d\zeta^2} + (\zeta')^{-2}\left(\frac{g''}{g} + \sigma^2 M(x, y)\right)w = 0.$$

Now taking

$$(\zeta')^{-2} M(x, y) = -\zeta,$$

We find the expression for ζ:

$$\begin{aligned} \zeta^{\frac{1}{2}}\zeta' &= \pm\sqrt{-M(x, y)} \\ \tfrac{2}{3}\zeta^{\frac{3}{2}} &= \pm\int^x \sqrt{-M(t, y)}dt \end{aligned} \tag{16}$$

and the one for $g(x)$, after inserting (16) into (15):

$$g(x) = \left(\frac{\zeta}{-M(x, y)}\right)^{\frac{1}{4}}.$$

Equation (14) now reduces to

$$\frac{d^2 w}{d\zeta^2} + \left(\frac{g''}{g'\zeta'^2} - \sigma^2\zeta\right) w = 0$$

which is satisfied by

$$w(\zeta) = w_0(\zeta) + \sum_{n=1}^{\infty} \sigma^{-2n} \left\{ a_n(\zeta) w_0(\zeta) + b_n(\zeta) \frac{dw_0}{d\zeta} \right\}.$$

where $w = w_0(\zeta)$ satisfies the differential equation

$$\frac{d^2 w}{d\zeta^2} - \sigma^2 \zeta w = 0 \tag{17}$$

and a_n and b_n can be found by successive approximations in orders of σ. (see D. S. Jones [4], pages 355–356).
If we restrict our attention to the first term of the series

$$w(\zeta) \approx w_0(\zeta),$$

our solution is an Airy function, as (17) shows.
Again $Bi\{\ldots\}$ is not satisfactory (exponential increase in region III), consequently

$$w(\zeta) = c\, Ai\{\sigma^{\frac{2}{3}} \zeta\}.$$

To sum up, the wave function is expressed by

$$\psi = c \left(\frac{\zeta}{-M(x, y)} \right)^{\frac{1}{4}} Ai\{\sigma^{\frac{2}{3}} \zeta\}, \tag{18}$$

an expression remaining bounded around the reversal point. In order to check wheather (18) agrees with the W.K.B. solution, away from $x = a$, $Ai\{\sigma^{\frac{2}{3}}\zeta\}$ must be expanded for large negative values of the argument (valid in the whole region except for a very small neighbourhood of $x = a$):

$$\psi = \frac{c}{\pi^{\frac{1}{2}}} M^{-\frac{1}{4}}(x, y) \sigma^{-\frac{1}{6}} \cos\left\{ \sigma \int^x \sqrt{M(t, y)}\, dt - \frac{\pi i}{4} \right\} \text{(see appendix B)}.$$

Taking only the incident wave, and choosing the constants in it in such a way that boundary condition $\psi_+(0) = C_1$ is fulfilled, we get

$$\psi_+ = \frac{C_1}{M^{\frac{1}{4}}(x, y)} \exp\left\{ i\sigma \int_0^x \sqrt{M(t, y)}\, dt \right\} \tag{19}$$

where

$$C_1 = \frac{c}{2\pi^{\frac{1}{2}}} \sigma^{-\frac{1}{6}} \exp\left(-\frac{\pi i}{4} \right).$$

The reversing wave similarly becomes

$$\psi_- = \frac{C_1}{M^{\frac{1}{4}}(x, y)} \exp\left\{ -i\sigma \int^x \sqrt{M(t, y)}\, dt \right\} \exp\left(-\frac{\pi i}{2} \right),$$

and if the boundary conditions for phase and modulus at $x = a$ are satisfied by defining the constants, we arrive at a formula which is in perfect agreement with eq. (13) of the W.K.B. method, just as (19) equals (12).

3. Solution, expanded with respect to B_1/E.
We simplify $M(x, y)$ as follows

$$M(x, y) = 1 - \frac{U_0(x)}{E} - \varepsilon\, e^{k(x-b)} \cos ky,$$

only using the first term of the series (8), with $\varepsilon = B_1/E$.
We get as phase of the incident wave

$$\int_0^x \sqrt{M(t, y)}\, dt = \int_0^x \left(\frac{a-t}{a} - \varepsilon\, e^{k(t-b)} \cos ky \right)^{\frac{1}{2}} dt. \tag{20}$$

If

$$\frac{a-x}{a} \gg \varepsilon \, e^{k(x-b)} \cos ky \tag{21}$$

the square root may be approximated by

$$\int_0^x \sqrt{M(t,y)}\,dt = \int_0^x \left(\frac{a-t}{a}\right)^{\frac{1}{2}} dt - \frac{\varepsilon}{2} \cos ky \int_0^x e^{k(t-b)} \sqrt{\frac{a}{a-t}}\, dt\,,$$

of which the last integral converts by integration by parts to

$$\int_0^x e^{k(t-b)} \sqrt{\frac{a}{a-t}}\, dt = e^{k(t-b)} k^{-1} \sqrt{\frac{a}{a-t}}\,\Bigg|_0^x - \int_0^x e^{k(t-b)} \sqrt{\frac{a}{a-t}} \frac{dt}{2k(a-t)}\,. \tag{22}$$

In the region where (21) holds, the second term of the right-hand side of (22) is very small because $k(a-x) \gg 1$. Consequently, we may write approximately

$$\int_0^x e^{k(t-b)} \sqrt{\frac{a}{a-t}}\, dt = k^{-1} \left(e^{k(x-b)} \sqrt{\frac{a}{a-x}} - e^{-kb} \right),$$

which changes (20) into

$$\int_0^x \sqrt{M(t,y)}\,dt = -\tfrac{2}{3} a \left\{ \left(\frac{a-x}{a}\right)^{\frac{3}{2}} - 1 \right\} - \frac{\varepsilon}{2k} \cos ky \left(e^{k(x-b)} \sqrt{\frac{a}{a-x}} - e^{-kb} \right). \tag{23}$$

Making a somewhat more rough estimation for the modulus

$$M(x,y)^{-\frac{1}{4}} = \left(\frac{a}{a-x}\right)^{\frac{1}{4}}, \tag{24}$$

we can combine (23) and (24), and find the complete formula for the incident wave

$$\psi_+^{\mathrm{II}} = C_1 \left(\frac{a}{a-x}\right)^{\frac{1}{4}} \exp\left[-\tfrac{2}{3} i\sigma a \left\{ \left(\frac{a-x}{a}\right)^{\frac{3}{2}} - 1 \right\} \right] \times$$

$$\exp\left\{ -i\sigma \frac{\varepsilon}{2k} \cos ky \left(e^{k(x-b)} \sqrt{\frac{a}{a-x}} - e^{-kb} \right) \right\}. \tag{25}$$

This result can be derived directly by means of the perturbation method. The returning wave has the same modulus function as the incident wave, and after applying a similar approximation of the square root, its phase becomes:

$$\left\{ \int_0^a - \int_a^x \right\} \sqrt{M(t,y)}\,dt =$$

$$= \left\{ 2\int_0^a - \int_0^x \right\} \left(\frac{a-t}{a}\right)^{\frac{1}{2}} dt - \frac{\varepsilon}{2} \cos ky \left\{ 2\int_0^a - \int_0^x \right\} e^{k(t-b)} \sqrt{\frac{a}{a-t}}\, dt\ . \tag{26}$$

The last integral in the right-hand term may be converted, like we did for the incident wave, into

$$-\int_0^x e^{k(x-b)} \sqrt{\frac{a}{a-t}}\, dt = -k^{-1} \left(e^{k(x-b)} \sqrt{\frac{a}{a-x}} - e^{-kb} \right). \tag{27}$$

However the last integral but one of (26), which has the same integrand as (27) but not the same boundaries, must be approached differently:

Substitution of

$$u = \sqrt{k(a-x)}$$

yields

$$\int_0^a e^{k(t-b)} \sqrt{\frac{a}{a-t}}\, dt = -2\, e^{k(x-b)} \sqrt{\frac{a}{k}} \int_{\sqrt{ka}}^{0} e^{-u^2}\, du\,,$$

and replacing the large number $\sqrt{ka}$ by ∞, we get approximately

$$-\int_{\sqrt{ka}}^{0} e^{-u^2} du = \int_0^{\infty} e^{-u^2} du\,,$$

which is Poisson's integral, known to have the value $\frac{1}{2}\sqrt{\pi}$, so that

$$\int_0^a e^{k(t-b)} \sqrt{\frac{a}{a-t}}\, dt = e^{k(a-b)} \sqrt{\frac{a\pi}{k}}\,.$$

Setting the integrals in (26), we obtain

$$\int_0^a - \int_a^x \sqrt{M(t, y)}\, dt = \tfrac{2}{3}a\left\{\left(\frac{a-x}{a}\right)^{\frac{3}{2}} + 1\right\} - \varepsilon \cos ky\, e^{k(a-b)} \sqrt{\frac{a\pi}{k}} + \\ + \frac{\varepsilon}{2k} \cos ky \left\{ e^{k(x-b)} \sqrt{\frac{a}{a-x}} - e^{-kb}\right\}$$

and using the correct constant with respect to the connection in $x=a$, it follows that the complete returning wave is

$$\psi_-^{\mathrm{II}} = C_1 \left(\frac{a}{a-x}\right)^{\frac{1}{4}} \exp\left[\tfrac{2}{3} i\sigma a \left\{\left(\frac{a-x}{a}\right)^{\frac{3}{2}} + 1\right\}\right] \exp\left(-i\sigma\varepsilon \cos ky\, e^{k(x-b)} \sqrt{\frac{a\pi}{k}}\right. \times \\ \times \exp\left\{ i\sigma \frac{\varepsilon}{2k} \cos ky \left(e^{k(x-b)} \sqrt{\frac{a}{a-x}} - e^{-kb}\right)\right\} \exp\left(-\frac{\pi i}{2}\right).$$

In region I the same procedure of approximating the square root can be followed

$$\int_0^x \sqrt{M(t, y)}\, dt = \int_0^x dt - \frac{\varepsilon}{2} \cos ky \int_0^x e^{k(t-b)} dt = \\ = x - \frac{\varepsilon}{2k} \cos ky \left(e^{k(x-b)} - e^{-kb}\right),$$

leading to

$$\psi_+^{\mathrm{I}} = C_1 \exp(i\sigma x) \exp\left\{ -i\sigma \frac{\varepsilon}{2k} \cos ky \left(e^{-k(x-b)} - e^{-kb}\right)\right\}, \tag{28}$$

and similarly we find

$$\psi_-^{\mathrm{I}} = C_1 \exp\{-i\sigma(x - \tfrac{4}{3}a)\} \exp\left\{-i\sigma\varepsilon \cos ky\, e^{k(a-b)} \sqrt{\frac{a\pi}{k}}\right\} \times \\ \times \exp\left\{ i\sigma \frac{\varepsilon}{2k} \cos ky \left(e^{k(x-b)} - e^{-kb}\right)\right\} \exp\left(-\frac{\pi i}{2}\right). \tag{29}$$

If we examine these results, we must conclude that

$$\psi_+^{\mathrm{I}} = C_1 \exp(i\sigma x) \tag{30}$$

$$\psi_-^{\mathrm{I}} = C_1 \exp\{-i\sigma(x - \tfrac{4}{3}a)\} \exp\left\{-i\sigma\varepsilon \cos ky\, e^{k(x-b)} \sqrt{\frac{a\pi}{k}}\right\} \exp\left(-\frac{\pi i}{2}\right) \tag{31}$$

are good approximations of (28) and (29), because of the extremely small value of $e^{k(x-b)}$ in region I.

4. Probability current density

The information about the specimen which is contained in the wave function in the form of a small perturbation, will become most easily observable by expressing it in the probability current density. Therefore we calculate ([5], [6]):

$$J(x) = \frac{i\hbar}{2m}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)$$

using the formulas

$$\psi_+ = C_1 M^{-\frac{1}{4}}(x, y)\exp\left\{i\sigma\int_0^x \sqrt{M(t, y)}dt\right\}$$

$$\psi_- = C_1 M^{-\frac{1}{4}}(x, y)\exp\left\{-i\sigma\int_p^x \sqrt{M(t, y)}dt\right\},$$

(p so to choose that the two formulas connect in $x=a$) and find

$$J_+(x) = \frac{C_1^2}{m}\hbar M^{-\frac{1}{2}}(x, y)\frac{\partial}{\partial x}\left\{\sigma\int_0^x \sqrt{M(t, y)}dt\right\} = C_1^2\sqrt{\frac{2E}{m}}$$

$$J_-(x) = -C_1^2\sqrt{\frac{2E}{m}}$$

independent of the presence of a specimen perturbation.

But in the case of the J in the y-direction, we get

$$J_+(y) = C_1^2\sqrt{\frac{2E}{m}}M^{-\frac{1}{2}}(x, y)\frac{\partial}{\partial y}\left\{\int_0^x \sqrt{M(t, y)}dt\right\}$$

$$J_-(y) = C_1^2\sqrt{\frac{2E}{m}}M^{-\frac{1}{2}}(x, y)\frac{\partial}{\partial y}\left\{-\int_p^x \sqrt{M(t, y)}dt\right\}. \tag{32}$$

As a result of taking

$$-\int_p^x \sqrt{M(t, y)}dt = -x - \frac{\varepsilon}{2k}\cos ky\, e^{k(x-b)}\sqrt{\frac{a\pi}{k}}$$

for the reversal beam in region I, (32) becomes

$$J_-^{\mathrm{I}}(y) = C_1^2\sqrt{\frac{2E}{m}}M^{-\frac{1}{2}}(x, y)\frac{\varepsilon}{2}\sin ky\, e^{k(x-b)}\sqrt{\frac{a\pi}{k}}.$$

This expression indeed elucidates the behaviour of the returning electron beam in region I in a very simple way, and although the formula is not obtained entirely correctly, it gives a good image of the actual phenomena. Moreover, it gives an indication of how the beam must have behaved near the reversal point, as fig. 3 shows.

The arrows in fig. 3 (r.h.s.), representing the probability current density in the y-direction, show that $J_-(y)=0$ in $y=0$, and $J_-(y)$ is maximum in $y=n\pi/k$.

Similar calculations of J, by using the more correct W.K.B. and Langer's results are far beyond the theoretical possibilities; however, they could be done numerically.

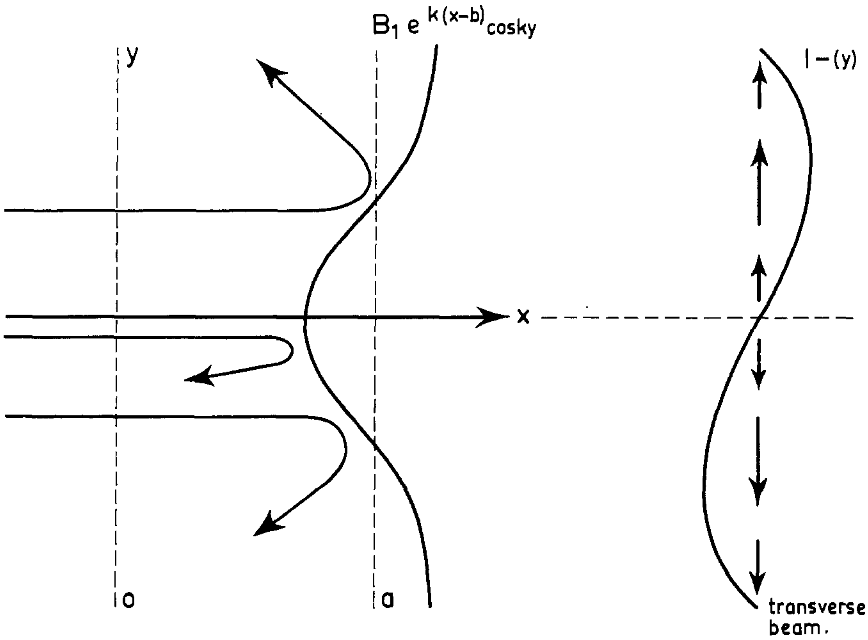

Figure 3. Reflection against equipotential plane curved by a first order sinusoidal perturbation.

Appendix A.

The assumption

$$\left|\frac{\partial^2 \psi}{\partial y^2}\right| \ll \left|\frac{\partial^2 \psi}{\partial x^2}\right| \tag{A1}$$

is still to be checked.

Using Langer's result (18) we can deduce

$$\frac{\partial^2 \psi}{\partial y^2} \approx c\left(\frac{\zeta}{-M(x, y)}\right)^{\frac{1}{4}} Ai''\{\sigma^{\frac{2}{3}}\zeta\} \cdot \sigma^{\frac{4}{3}}\left(\frac{\partial \zeta}{\partial y}\right)^2$$

$$\frac{\partial^2 \psi}{\partial x^2} \approx c\left(\frac{\zeta}{-M(x, y)}\right)^{\frac{1}{4}} Ai''\{\sigma^{\frac{2}{3}}\zeta\} \cdot \sigma^{\frac{4}{3}}\left(\frac{\partial \zeta}{\partial x}\right)^2$$

which is a good approximation for $a-x$ sufficiently large, so that (A1) converts into

$$\left|\frac{\partial \zeta}{\partial y}\right| \ll \left|\frac{\partial \zeta}{\partial x}\right| . \tag{A2}$$

It follows from (16) that we may replace (A2) by

$$\left|\frac{\partial}{\partial y}\int^{x} \sqrt{M(t, y)}\, dt\right| \ll \left|\sqrt{M(x,y)}\right| . \tag{A3}$$

Investigating

$$M(x, y) = 1 - \frac{U_0(x)}{E} - \varepsilon f(x, y),$$

$f(x, y)$ standing for the series of perturbation terms, and finding that apart from $x=a$

$$1 - \frac{U_0(x)}{E} \gg \varepsilon f(x, y),$$

we clearly see that for any arbitrary small distance from $x=a$, ε can be chosen such that (A3) is satisfied. However, statement (A1) is not proven around the reversal point.

Appendix B: Airy Functions

The differential equation

$$w''(z) - z \cdot w(z) = 0$$

possesses two linear independent solutions, called the Airy functions of the first and second kind, [1], [3], [4]:

$$Ai(z) = \frac{1}{2\pi i} \int_l \exp(zu - \tfrac{1}{3}u^3)\, du \tag{B1}$$

$$Bi(z) = i \exp(-\tfrac{2}{3}\pi i) Ai\{z \exp(-\tfrac{2}{3}\pi i)\} - i \exp(\tfrac{2}{3}\pi i) Ai\{z \exp(\tfrac{2}{3}\pi i)\} \tag{B2}$$

hence the integration path l runs from $u = \infty \cdot \exp(-\tfrac{2}{3}\pi i)$ to $u = \infty \cdot \exp(\tfrac{2}{3}\pi i)$. Both these solutions represent a linear combination of Bessel functions of order 1/3.

In the case of large positive values of their argument z, the Airy functions are expressed by an asymptotic representation

$$Ai(z) \sim \frac{1}{2\pi^{\frac{1}{2}}} z^{-\frac{1}{4}} \exp(-\tfrac{2}{3} z^{\frac{3}{2}})$$

$$Bi(z) \sim \frac{1}{\pi^{\frac{1}{2}}} z^{-\frac{1}{4}} \exp(\tfrac{2}{3} z^{\frac{3}{2}})$$

and for large negative values of z

$$Ai(z) \sim \frac{1}{\pi^{\frac{1}{2}}} |z|^{-\frac{1}{4}} \cos\left(\frac{2}{3}|z|^{\frac{3}{2}} - \frac{\pi}{4}\right)$$

$$Bi(z) \sim \frac{-1}{\pi^{\frac{1}{2}}} |z|^{-\frac{1}{4}} \sin(\tfrac{2}{3}|z|^{\frac{3}{2}}) .$$

The behaviour of the solutions in the so-called transition region, where z has a small value, appears from the Taylor series of (B1) and (B2)

$$Ai(z) = \frac{3^{-\frac{2}{3}}}{\pi} \sum_{n=0}^{\infty} \frac{1}{n!} \Gamma\left(\frac{n+1}{3}\right) \sin\{\tfrac{2}{3}(n+1)\pi\}(3^{\frac{1}{3}}z)^n$$

$$Bi(z) = \frac{3^{-\frac{2}{3}}}{2\pi} \sum_{n=0}^{\infty} \Gamma\left(\frac{n+1}{3}\right) \frac{1}{n!} \sin^2\{\tfrac{2}{3}(n+1)\pi\}(3^{\frac{1}{3}}z)^n ,$$

or written differently

$$Ai(z) = c_1 f(z) - c_2 g(z)$$

$$Bi(z) = \sqrt{3}\{c_1 f(z) + c_2 g(z)\} ,$$

hence

$$f(z) = 1 + \frac{1}{3!} z^3 + \frac{1 \cdot 4}{6!} z^6 + \frac{1 \cdot 4 \cdot 7}{9!} z^9 + \ldots = \sum_{n=0}^{\infty} 3^n (\tfrac{1}{3})_n \frac{z^{3n}}{(3n)!}$$

$$g(z) = z + \frac{2}{4!} z^4 + \frac{2 \cdot 5}{7!} z^7 + \frac{2 \cdot 5 \cdot 8}{10!} z^{10} + \ldots = \sum_{n=0}^{\infty} 3^n (\tfrac{2}{3})_n \frac{z^{3n+1}}{(3n+1)!}$$

$$C_1 = Ai(0) = \frac{Bi(0)}{\sqrt{3}} = \frac{3^{-\frac{2}{3}}}{\Gamma(\frac{2}{3})}$$

$$C_2 = -Ai'(0) = \frac{Bi(0)}{\sqrt{3}} = \frac{3^{-\frac{1}{3}}}{\Gamma(\frac{1}{3})}$$

whereas $Ai(0)$ and $Ai'(0)$ are the values of the Airy function and its derivative in the transition point.

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