PHYSICAL REVIEW B VOLUME 2, NUMBER 6 15 SEPTEMBER 1970

Impurity-Assisted Inelastic Tunneling: One-Electron Theory

A. D. Brailsford and L. C. Davis
Scientific Research Staff, Ford Motor Company, Dearborn, Michigan 48121
(Received 27 March 1970)

A new theory of inelastic tunneling through insulating barriers containing impurities with vibrational modes is presented. The method is based upon a stationary-state formulation of the problem, and is a direct extension of the conventional treatment of elastic tunneling which appears in standard texts. In this paper the inelastic processes for one electron are studied in first Born approximation and compared with the results for a model interaction which can be solved exactly. The physical implications of the treatment are discussed and certain results are established for later use in the many-electron theory to be presented in the following paper.

I. INTRODUCTION

Inelastic-tunneling processes involving the excitation of vibrational modes of molecular impurities in the insulating barrier of a metal-insulator-metal tunnel juction were discovered and identified by Jaklevic and Lambe.[1,2] Experimentally, each such process is manifested as a narrow peak in a plot of the derivative of the conductance with respect to voltage versus voltage at the value $eV = \hbar\omega$, where $\hbar\omega$ is the excitation energy of the mode. It occurs because beyond the threshold voltage it is possible for an electron to tunnel from one metal through the barrier, give up energy $\hbar\omega$ to the impurity en route, and still have sufficient energy to find an unoccupied state in the other metal electrode. The onset of this additional channel produces a (roughly) linear increase in current with voltage, and hence a peak in the second derivative.

Following the initial explanation, Scalapino and Marcus[3] formulated a theory of the process by incorporating within the WKB approximation the dipole potential (plus image) of the molecule for infrared-active modes. This approach was later extended by Lambe and Jaklevic[2] to include Raman-active modes. More recently, Duke[4] has discussed the problem in terms of the transfer Hamiltonian formalism, the inelastic channel being viewed as a transition, from a left-hand-metal state to a right-hand-metal state, whose strength (i.e., matrix element) is determined by the overlap of the product of a left- and right-hand state with the potential of Scalapino and Marcus.

Both of these methods are able to account satisfactorily for the experimental observations. Nevertheless, it appears that they are unnecessarily approximate in their treatment of the inelastic process. The WKB approach necessitates the validity of the adiabatic approximation for computing impurity-assisted barrier-penetration factors, whereas, the transfer-Hamiltonian approach entails approximations in its formulation which are discussed extensively by Duke.[5] The purpose of this and the following paper is to present a theory of inelastic tunneling which is free from these deficiencies. It is based upon orthogonal current-carrying states which are eigenfunctions of the entire noninteracting one-electron system (it does not depend upon the construction of model left- and right-hand systems) and treats the coupling to the impurity without appeal to the adiabatic hypothesis. In addition, the method allows us to examine the modifications in the elastic-channel current due to energy-loss mechanisms in the barrier, an effect which is not encompassed by other theories of the over-all tunneling process.

The theory is derived for a square-barrier potential and arbitrary interaction potential, but our main applications are to a one-dimensional square barrier with the impurity interaction confined to within the barrier region. We consider a "vibrator" as giving rise to the energy-loss mechanism, this being representative of a molecular impurity or, in general, of phonons, magnetic impurities in a magnetic field, etc. The analysis can be generalized to include impurity interactions extending beyond the barrier regions and to three dimensions in a straightforward manner.

Our method is essentially an extension of conventional treatments of tunneling using stationary eigenstates[6] in which we include the dynamics of the scattering centers. For the one-electron problem this can be achieved readily by adapting standard techniques of inelastic scattering[7] to the problem. Unfortunately, this is still far from experiment since the Fermi statistics obviously play a vital role in determining the threshold behavior of the inelastic process. Consequently, it is necessary to extend the analysis to a many-

electron system. This has proved to be a considerable undertaking requiring extensive analysis. For this reason, and because the method is new and may have separate application outside the scope of the present problem, it is presented separately in the following paper.[8] The present manuscript deals exclusively with the one-electron aspects of the theory. These are a necessary prerequisite for understanding the many-electron problem and allow us to analyze some of the approximations which seem unavoidable in the latter case.

The paper is organized as follows. In the Sec. II we formulate the one-electron problem in terms of stationary eigenstates and derive the first-order Born-approximation result for a fairly general impurity interaction (its main characteristics are defined in the text). This scheme is essential to the development in II and, consequently, in Sec. III we compare the results of the method with those for a model impurity potential for which the exact solution is derived. Finally, in Sec. IV we discuss the physical content of the method in relation to the stationary states we have obtained. This concludes the preparatory study for the many-electron treatment in II.

II. BORN APPROXIMATION

In this section we consider one electron interacting with a vibrator in a potential barrier. We restrict the electron to one-dimensional motion perpendicular to the barrier (x direction) and denote the coordinate describing the internal motion of the vibrator by ξ.

The Hamiltonian for the system is given by

$$\mathcal{H}(x,\xi)=\mathcal{H}_e(x)+\mathcal{H}_v(\xi)+\mathcal{H}_{ev}(x,\xi) \quad , \tag{2.1}$$

where

$$\mathcal{H}_e(x)=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x) \quad . \tag{2.2}$$

For simplicity we consider only a square barrier, i.e., $V(x)=V_0$ for $0<x<b$ and $V(x)=0$ otherwise. The Hamiltonian for the vibrator is $H_v(\xi)$ and the interaction of the electron with the vibrator is denoted by $\mathcal{H}_{ev}(x,\xi)$. We assume that the eigenfunctions of $\mathcal{H}_v(\xi)$ are known,

$$\mathcal{H}_v(\xi)\Phi_n(\xi)=E_{vn}\Phi_n(\xi) \quad . \tag{2.3}$$

The electron-vibrator coupled system is closed, so that stationary states of $\mathcal{H}(x,\xi)$ can be found,

$$\mathcal{H}(x,\xi)\Psi(x,\xi)=E\Psi(x,\xi) \quad . \tag{2.4}$$

We can expand $\Psi(x,\xi)$ in terms of the complete set $\Phi_n(\xi)$ as follows:

$$\Psi(x,\xi)=\textstyle\sum_n \chi_n(x)\Phi_n(\xi) \quad . \tag{2.5}$$

We further simplify the problem by retaining only two terms in Eq. (2.5) corresponding to the ground state and the first excited state of the vibrator, since this is sufficient to encompass the inelastic-tunneling processes of current interest. (Furthermore, it would entail no approximation were the vibrator a magnetic impurity of spin $\frac{1}{2}$.) Thus, denoting the ground state of the vibrator by $\Phi_0(\xi)$ and the first excited state by $\Phi_1(\xi)$, Eq. (2.5) becomes

$$\Psi(x,\xi)=\chi_0(x)\Phi_0(\xi)+\chi_1(x)\Phi_1(\xi) \quad , \tag{2.6}$$

and upon substituting Eq. (2.6) into (2.4), we find the following coupled equations for $\chi_0(x)$ and $\chi_1(x)$:

$$\mathcal{H}_e(x)\chi_0(x)+U(x)\chi_1(x)=\epsilon\chi_0(x) \quad , \tag{2.7a}$$

$$\mathcal{H}_e(x)\chi_1(x)+U(x)\chi_0(x)=(\epsilon-\hbar\omega)\chi_1(x) \quad , \tag{2.7b}$$

where

$$U(x)=\int d\xi\, \Phi_1^*(\xi)\mathcal{H}_{ev}(x,\xi)\Phi_0(\xi) \quad , \tag{2.8a}$$

$$\epsilon=E-E_{v0} \quad , \tag{2.8b}$$

and

$$\hbar\omega=E_{v1}-E_{v0} \quad . \tag{2.8c}$$

In the case of molecular vibrations, the interaction potential $U(x)$ is a dipole potential plus its image.[3] In general, it will be real as assumed in (2.7). Terms such as $\int d\xi\, \Phi_0^*(\xi)\mathcal{H}_{ev}(x,\xi)\Phi_0(\xi)$, which are additional static potentials, are of no interest here and have been omitted.

We first solve Eq. (2.7) approximately for a small, but otherwise arbitrary, interaction potential $U(x)$. The accuracy of our approximation is tested in Sec. III by comparing with the exact results for a model potential. We use notation which allows us to extend the results of this section to the many-electron system considered in Paper II.

To zeroth order in U, we have

$$[\mathcal{H}_e(x)-\epsilon]\chi_0^{(0)}(x)=0 \quad , \tag{2.9}$$

which has the solution

$$\chi_0^{(0)}(x)=\psi(x) \quad , \tag{2.10}$$

where

$$\begin{aligned}\psi(x)&=e^{ikx}+Re^{-ikx}, && x<0\\ &=Ce^{-Kx}+De^{Kx}, && 0<x<b\\ &=Te^{ik(x-b)}, && b<x\end{aligned} \tag{2.11a}$$

with

$$R=\frac{k-iK}{2k}(1-e^{-2Kb})C \quad , \tag{2.11b}$$

$$D=-\frac{k-iK}{k+iK}e^{-2Kb}C \quad , \tag{2.11c}$$

$$T = \frac{2iK}{k+iK} e^{-Kb} C \quad , \tag{2.11d}$$

$$C = \frac{2k}{k+iK}\left[1 - \left(\frac{k-iK}{k+iK}\right)^2 e^{-2Kb}\right]^{-1} \quad , \tag{2.11e}$$

$$k = (2m\epsilon/\hbar^2)^{1/2} \quad , \tag{2.11f}$$

and

$$K = [2m(V_0 - \epsilon)/\hbar^2]^{1/2} \quad . \tag{2.11g}$$

We have chosen boundary conditions corresponding to an electron incident on the barrier from the left. There is also a solution obtained from Eq. (2.11) by replacing x by $b - x$. Such a solution corresponds to an electron incident from the right. Similarly, to first order in U, we have

$$[\mathcal{H}_e(x) - \epsilon + \hbar\omega]\chi_1^{(1)}(x) = -U(x)\chi_0^{(0)}(x) \quad . \tag{2.12a}$$

To simplify the notation, we write $\chi_1^{(1)}(x) = \psi'(x)$. Then, Eq. (2.12a) has the solution

$$\psi'(x) = \int dx' K(\epsilon - \hbar\omega, x, x')U(x')\psi(x') \quad , \tag{2.12b}$$

where the Green's function $K(\epsilon, x, x')$ satisfies

$$[\mathcal{H}_e(x) - \epsilon]K(\epsilon, x, x') = -\delta(x - x') \quad . \tag{2.13}$$

Since we are restricting our attention to cases where $U(x)$ vanishes outside the barrier, we need to find $K(\epsilon, x, x')$ only for $0 < x' < b$. In this case the solution of (2.13) is

$$\begin{aligned} K(\epsilon, x, x') &= r(\epsilon, x')e^{-ikx}, && x < 0 \\ &= c(\epsilon, x')e^{-Kx} + d(\epsilon, x')e^{Kx}, && 0 < x < x' \\ &= f(\epsilon, x')e^{-Kx} + g(\epsilon, x')e^{Kx}, && x' < x < b \\ &= t(\epsilon, x')e^{ik(x-b)} \quad , && b < x \end{aligned} \tag{2.14a}$$

where the functions $r(\epsilon, x')$, etc., are found to be given by

$$r(\epsilon, x') = -\frac{2iK}{k-iK} c(\epsilon, x') \quad , \tag{2.14b}$$

$$d(\epsilon, x') = -\frac{k+iK}{k-iK} c(\epsilon, x') \quad , \tag{2.14c}$$

$$g(\epsilon, x') = -\frac{k-iK}{k+iK} e^{-2Kb} f(\epsilon, x') \quad , \tag{2.14d}$$

$$t(\epsilon, x') = \frac{2iK}{k+iK} e^{-Kb} f(\epsilon, x') \quad , \tag{2.14e}$$

$$c(\epsilon, x') = \left(\frac{k-iK}{k+iK}\right)\left(\frac{m}{\hbar^2 K}\right) e^{-Kx'}\left[1 - \left(\frac{k-iK}{k+iK}\right)e^{-2K(b-x')}\right] \times \left[1 - \left(\frac{k-iK}{k+iK}\right)^2 e^{-2Kb}\right]^{-1} \quad , \tag{2.14f}$$

$$f(\epsilon, x') = -\frac{m}{\hbar^2 K}\left[e^{Kx'} - \left(\frac{k-iK}{k+iK}\right)e^{-Kx'}\right] \times \left[1 - \left(\frac{k-iK}{k+iK}\right)^2 e^{-2Kb}\right]^{-1} \quad , \tag{2.14g}$$

$$k = (2m\epsilon/\hbar^2)^{1/2} \quad , \tag{2.14h}$$

and

$$K = [2m(V_0 - \epsilon)/\hbar^2]^{1/2} \quad . \tag{2.14j}$$

The above result is obtained by requiring the continuity of $K(\epsilon, x, x')$ and $(\partial/\partial x)K(\epsilon, x, x')$ at $x = 0$ and $x = b$, by requiring that $K(\epsilon, x, x')$ is continuous at $x = x'$, and that

$$\left.\frac{\partial K(\epsilon, x, x')}{\partial x}\right|_{x=x'-0^+}^{x=x'+0^+} = \frac{2m}{\hbar^2} \quad ,$$

this last condition being obtained by integrating (2.13) over a vanishingly small interval centered at $x = x'$. Furthermore, we have required that $K(\epsilon, x, x')$ obey the boundary condition of an outgoing wave. Thus, from Eq. (2.14), we see that

$$\psi'(x) = R'e^{-ik'x}, \qquad x < 0 \tag{2.15a}$$

and

$$= T'e^{ik'(x-b)}, \quad b < x \tag{2.15b}$$

where

$$R' = \int_0^b dx' r(\epsilon - \hbar\omega, x')U(x')\psi(x') \quad , \tag{2.15c}$$

$$T' = \int_0^b dx' t(\epsilon - \hbar\omega, x')U(x')\psi(x') \quad , \tag{2.15d}$$

and

$$k' = [2m(\epsilon - \hbar\omega)/\hbar^2]^{1/2} \quad . \tag{2.15e}$$

The wave function for the system is then

$$\psi(x, \xi) = \chi_0^{(0)}(x)\Phi_0(\xi) + \chi_1^{(1)}(x)\Phi_1(\xi) \tag{2.16a}$$

$$= \psi(x)\Phi_0(\xi) + \psi'(x)\Phi_1(\xi) \quad , \tag{2.16b}$$

in first order. We have chosen boundary conditions corresponding to the following situation. When an electron is incident upon the barrier, the vibrator is in the ground state. The electron can be elastically reflected or elastically transmitted, the vibrator remaining unexcited. This is represented by $\psi(x)\Phi_0(\xi)$ in Eq. (2.16b). In addition, the electron can excite the vibrator by being inelastically reflected or inelastically transmitted. In this case the electron loses energy $\hbar\omega$ to the vibrator. This is represented by $\psi'(x)\Phi_1(\xi)$ in Eq. (2.16b). The amplitude for elastic reflection is R, elastic transmission T, inelastic reflection R', and inelastic transmission T'.

Equation (2.16) is the wave function for the system in first Born approximation. We could proceed in a similar manner to obtain second- and higher-order Born approximations. We will not do this now although we show in Sec. III that it is essential if one is to obtain the elastic-tunnel current to order U^2, which is required in Paper II.

III. EXACT SOLUTIONS FOR MODEL INTERACTION POTENTIAL

Since the Born approximation is the basis of the many-electron treatment it is desirable to check its accuracy and also to examine some of the qualitative features of inelastic tunneling for an exactly soluble problem. Accordingly, in this section we analyze the solution of (2.7) for a model interaction potential $U(x)$ given by

$$\begin{aligned} U(x) &= 0\,, && x < x_1 \\ &= U_0, && x_1 < x < x_2 \\ &= 0\,, && x_2 < x \end{aligned} \tag{3.1}$$

where $0 \le x_1 < x_2 \le b$.

Outside the barrier ($x < 0$ and $x > b$) particular solutions of Eq. (2.7) are of the form

$$\chi_0(x) = e^{\pm ikx}, \quad k = (2m\epsilon/\hbar^2)^{1/2}\,, \tag{3.2a}$$

$$\chi_1(x) = e^{\pm ik'x}, \quad k' = [2m(\epsilon - \hbar\omega)/\hbar^2]^{1/2}\,; \tag{3.2b}$$

whereas, inside the barrier, in the regions where $U(x) = 0 (0 < x < x_1$ and $x_2 < x < b)$, particular solutions are

$$\chi_0(x) = e^{\pm Kx}, \quad K = [2m(V_0 - \epsilon)/\hbar^2]^{1/2}\,, \tag{3.3a}$$

and

$$\chi_1(x) = e^{\pm K'x}, \quad K' = [2m(V_0 - \epsilon + \hbar\omega)/\hbar^2]\,. \tag{3.3b}$$

In the region of interaction ($x_1 < x < x_2$) we note that a solution of the type

$$\chi_1(x) = \lambda\chi_0(x) \tag{3.4}$$

is possible, since $U(x)$ is constant in this region. Substituting Eq. (3.4) into Eq. (2.7), we find such particular solutions exist when

$$\lambda = \lambda_{1,2} = \{\hbar\omega \pm [(\hbar\omega)^2 + 4U_0^2]^{1/2}\}/2U_0 \tag{3.5}$$

and are of the form

$$\chi_0(x) = e^{\pm Qx}, \quad Q = \left[2m\left(V_0 - \epsilon + \frac{\lambda^2\hbar\omega}{\lambda^2 - 1}\right)\Big/\hbar^2\right]^{1/2}\,, \tag{3.6}$$

and $\chi_1(x)$ is given by Eq. (3.4) for each value of λ. We let $Q = Q_1$ for $\lambda = \lambda_1$, and $Q = Q_2$ for $\lambda = \lambda_2$. In the limit of small $U_0/\hbar\omega$, $Q_1 \to K'$ and $Q_2 \to K$ [see Eq. (3.3)]. For a wave (incoming) from the left, the general solution of Eq. (2.7) is then

$$\begin{aligned} \chi_0(x) &= e^{ikx} + Re^{-ikx}, && x < 0 \\ &= Ae^{-Kx} + Be^{Kx}, && 0 < x < x_1 \\ &= C_1e^{-Q_1x} + D_1e^{Q_1x} + C_2e^{-Q_2x} + D_2e^{Q_2x}, \\ &= Fe^{-Kx} + Ge^{Kx}, && x_1 < x < x_2 \\ &= Te^{ik(x-b)}, && x_2 < x < b \\ & && b < x \end{aligned} \tag{3.7a}$$

and

$$\begin{aligned} \chi_1(x) &= R'e^{-ik'x}, && x < 0 \\ &= A'e^{-K'x} + B'e^{K'x}, && 0 < x < x_1 \\ &= \lambda_1(C_1e^{-Q_1x} + D_1e^{Q_1x}) + \lambda_2(C_2e^{-Q_2x} + D_2e^{Q_2x}), \\ &= F'e^{-K'x} + G'e^{K'x}, && x_1 < x < x_2 \\ &= T'e^{ik'(x-b)}, && x_2 < x < b \\ & && b < x\,. \end{aligned} \tag{3.7b}$$

By requiring the continuity of $\chi_0(x)$, $d\chi_0/dx$, $\chi_1(x)$, and $d\chi_1/dx$ at $x = 0$, x_1, x_2, and b, we obtain 16 equations to determine the 16 unknowns (i.e., R, A, B, ...) in Eqs. (3.7). In general, these 16 linear simultaneous equations are most easily solved numerically.

In Fig. 1, some typical results are shown for parameters characteristic of a metal-insulator-metal junction and for an electron incident from the left. The inelastic-transmission probability

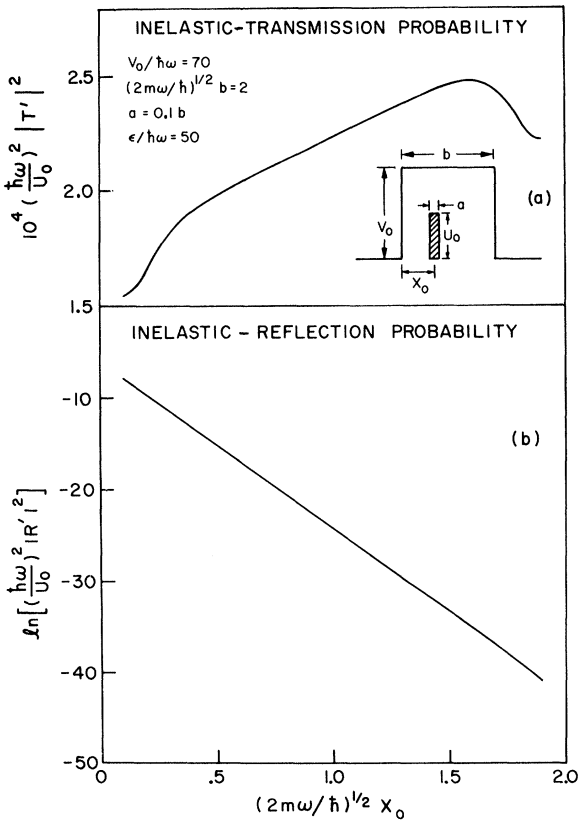

FIG. 1. (a) Inelastic-transmission probability $|T'|^2$ as a function of x_0, the distance of the vibrator from the leading edge of the barrier. The interaction potential is the model potential of Sec. III. (b) The logarithm of the inelastic-reflection coefficient $|R'|^2$ versus x_0. The results for both $|T'|^2$ and $|R'|^2$ scale with U_0^2 accurately for $(U_0/\hbar\omega) < 1$.

$|T'|^2$ and inelastic-reflection probability $|R'|^2$ are plotted as a function of the distance of the vibrator x_0 from the leading edge of the barrier. We have found that the results scale with U_0^2 to better than 1% over a wide range of parameters when $U_0/\hbar\omega < 1$. Calculations of $|T'|^2$ and $|R'|^2$ in first Born approximation agree with the exact results over the same range of parameters, which confirms the validity of the first Born approximation in this regime.

The inelastic-transmission probability increases slowly as the position of the vibrator is changed from $x_0 \simeq 0$ to $x_0 \simeq b$, except for a small region near b. Somewhat larger relative changes in $|T'|^2$ versus x_0 can be found for lower wider barriers. In contrast to this, the results for the inelastic-reflection probability $|R'|^2$ indicate a nearly exponential decrease with increasing x_0 for an electron incident from the left.

We can understand these results by examining Fig. 2, where $\chi_0(x)$ and $\chi_1(x)$ are shown schematically. An electron impinges on the barrier from the left at energy ϵ according to the boundary conditions imposed upon $\chi_0(x)$ [see Eq. (2.23a), $x < 0$]. Most of the incoming wave is reflected, but a small portion is transmitted elastically to the right due to the penetration of the wave function into the barrier. The vibrator acts as a source at x_0 for the inelastic wave function $\chi_1(x)$, which is an outgoing wave beyond the barrier region at energy $\epsilon - \hbar\omega$. The inelastically transmitted part results from an electron going from 0 to x_0 with energy ϵ, being scattered at x_0 by the vibrator, and going from x_0 to b with energy $\epsilon - \hbar\omega$. Since the electron suffers less attenuation with energy ϵ than with $\epsilon - \hbar\omega$, $|T'|^2$ will be larger the closer x_0 is to b, except for $x_0 \simeq b$ where more detailed considerations of the wave functions must be made. On the other hand, the inelastically reflected part results from an electron going from 0 to x_0 with energy ϵ, being scattered at x_0, and going from x_0 back to 0 with energy $\epsilon - \hbar\omega$. The exponential decrease of $|R'|^2$ with increasing x_0 is due to the attenuation of the electron going from 0 to x_0 with energy ϵ and going from x_0 back to 0 with energy $\epsilon - \hbar\omega$.

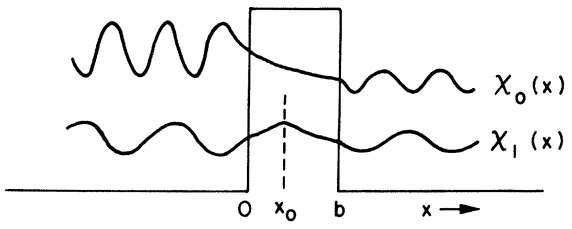

FIG. 2. Elastic wave function χ_0 corresponds to a wave incident from the left which is partially reflected to the left and partially transmitted to the right. The inelastic wave function χ_1 represents an outgoing wave with a source for the wave at the position of the vibrator x_0.

IV. DISCUSSION OF STATIONARY-STATE METHOD

In Secs. II and III we have shown that the stationary-state method provides a description of inelastic tunneling, and through the exact solution of a model problem, we have shown that the first-Born-approximation treatment is adequate for the inelastic channel for the range of parameters of physical interest. Certain conservation conditions are inherent in the coupled equations (2.7) which are important in the physical interpretation of this method. In this section these conditions are derived and analyzed.

The first condition must clearly be that the number of particles is conserved. This follows from the initial equations (2.7). Let $x_l < 0$ be a point to the left of the barrier and $x_r > b$ be a point to the right. Multiplying Eq. (2.7a) by $\chi_0^*(x)$ and integrating from x_l to x_r, we find

$$\int_{x_l}^{x_r} dx\, \chi_0^*(x)[\mathcal{H}_e(x) - \epsilon]\chi_0(x) = -\int_0^b dx\, \chi_0^*(x) U(x) \chi_1(x). \tag{4.1}$$

Subtracting the complex conjugate of Eq. (4.1) from Eq. (4.1), we have

$$-\frac{\hbar^2}{2m}\int_{x_l}^{x_r} dx \left(\chi_0^*(x)\frac{d^2\chi_0(x)}{dx^2} - \chi_0(x)\frac{d^2\chi_0^*(x)}{dx^2}\right) = -\int_0^b dx\, U(x)[\chi_0^*(x)\chi_1(x) - \chi_0(x)\chi_1^*(x)] \,. \tag{4.2}$$

Integrating by parts gives

$$-\frac{\hbar^2}{2m}\left(\chi_0^*(x)\frac{d\chi_0(x)}{dx} - \chi_0(x)\frac{d\chi_0^*(x)}{dx}\right)_{x_l}^{x_r} = -\int_0^b dx\, U(x)[\chi_0^*(x)\chi_1(x) - \chi_0(x)\chi_1^*(x)] \,. \tag{4.3}$$

Similarly, from Eq. (2.7b), we find

$$-\frac{\hbar^2}{2m}\left(\chi_1^*(x)\frac{d\chi_1(x)}{dx} - \chi_1(x)\frac{d\chi_1^*(x)}{dx}\right)_{x_l}^{x_r} = -\int_0^b dx\, U(x)[\chi_1^*(x)\chi_0(x) - \chi_1(x)\chi_0^*(x)] \,. \tag{4.4}$$

Thus, adding Eqs. (4.3) and (4.4) gives conservation of current across the barrier,

$$J(x_r) = J(x_l) \,, \tag{4.5a}$$

where

$$J(x) = -\frac{i\hbar}{2m}\left(\chi_0^*(x)\frac{d\chi_0(x)}{dx} - \chi_0(x)\frac{d\chi_0^*(x)}{dx}\right)$$

$$-\frac{i\hbar}{2m}\left(\chi_1^*(x)\frac{d\chi_1(x)}{dx}-\chi_1(x)\frac{d\chi_1^*(x)}{dx}\right) . \quad (4.5b)$$

Now, for any interaction potential $U(x)$, the asymptotic form of $\chi_0(x)$ and $\chi_1(x)$ will be the same as in Eq. (3.7). From Eq. (4.5), we have therefore

$$\frac{\hbar k}{m}|T|^2+\frac{\hbar k'}{m}|T'|^2=\frac{\hbar k}{m}-\frac{\hbar k}{m}|R|^2-\frac{\hbar k'}{m}|R'|^2 . \quad (4.6)$$

We note that if R' and T' are found in first Born approximation, they give a contribution to the current of order U^2, this being the lowest order in which the vibrator affects the current. Therefore, we must also calculate R and T through second Born approximation for current conservation to hold through order U^2. This is of importance in connection with the further analysis of Paper II.

The second condition is related to the energy flux. To the right of the barrier this is

$$J_{Er}=\frac{\hbar k}{m}\epsilon|T|^2+\frac{\hbar k'}{m}(\epsilon-\hbar\omega)|T'|^2 , \quad (4.7)$$

and to the left,

$$J_{El}=\frac{\hbar k}{m}\epsilon-\frac{\hbar k}{m}\epsilon|R|^2-\frac{\hbar k'}{m}(\epsilon-\hbar\omega)|R'|^2 . \quad (4.8)$$

Now by making use of Eq. (4.6), we find

$$J_{El}-J_{Er}=\frac{\hbar k'}{m}\hbar\omega(|T'|^2+|R'|^2) . \quad (4.9)$$

This represents the power absorbed by the vibrator as it makes transitions from its ground state to the first excited state. At first sight this presents a paradox, for how can such a situation lead to a stationary state? The resolution lies in our use of the boundary condition for the incident wave; for if we interpret the χ's as describing beams of particles, it is implicit in our use of an incident wave with $\Phi_0(\xi)$ only, that the vibrator be in contact with a heat sink which reverts the vibrator to its ground state after each inelastic event. It is only because it is possible to idealize this situation in terms of a boundary condition that the stationary-state method can describe inelastic processes. Naturally this idealization ignores the possibility that the excited vibrator energy levels may be broadened as a result of this interaction with the thermal bath but this effect is regarded as extraneous in the present context.

Probably the best physical picture is obtained by imagining a wave packet made up of these states. Such a wave packet would approach the barrier from the left with the vibrator in the ground state. After the wave packet has been scattered from the barrier, measurements of the position of the electron would reveal there is a probability of $|R|^2$ that the electron was elastically reflected and of $|T|^2$ it was elastically transmitted, the vibrator remaining in the ground state. Concomitantly, one would find a probability $|R'|^2$ that the electron was reflected inelastically with the vibrator making a transition from the ground state to the excited state, and a probability $|T'|^2$ that the electron was transmitted with excitation of the vibrator.

In summary, we have formulated a theory of inelastic tunneling of one electron in terms of the stationary states of the coupled electron-vibrator system. The resultant coupled equations for the elastic and inelastic electron wave functions were solved in first Born approximation. The results of first Born approximation were found to be quite accurate by comparing to the results of an exact model calculation. This one-electron theory forms the background for the many-electron theory given in II.

---

[1]R. C. Jaklevic and J. Lambe, Phys. Rev. Letters 17, 1139 (1966).

[2]J. Lambe and R. C. Jaklevic, Phys. Rev. 165, 821 (1968).

[3]D. J. Scalapino and S. M. Marcus, Phys. Rev. Letters 18, 459 (1967).

[4]C. B. Duke, *Tunneling in Solids* (Academic, New York, 1969), p. 290.

[5]See Ref. 4, p. 207.

[6]L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1949), Chap. 5.

[7]N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford U. P., London, 1965), 3rd ed., p. 327.

[8]L. C. Davis, following paper, Phys. Rev. B 2, 1714 (1970), hereafter referred to as II.