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ON THE THEORY OF INELASTIC SCATTERING OF SLOW ELECTRONS BY SURFACE EXCITATIONS: 1. HALF-SPACE FORMALISM *

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ABSTRACT

A quantum-mechanical theory for the inelastic scattering of slow electrons (ISSE) by surface excitations is developed within the half-space model. The process of transmission of incident electrons into the crystal is described by the homogeneous Schrödinger equation, while the scattering process inside the crystal is described by an inhomogeneous Schrödinger equation. The scattering cross-section for ISSE by surface excitations is derived and is found to be small since it is dependent on an inverse sum of wavevectors which is large. It is also dependent on the fluctuations in the scattering potential.

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I. INTRODUCTION

Inelastic scattering of slow electrons (ISSE) by surface excitations, should, in principle, be a powerful tool for the study of surface excitations. However, very few papers report on such a spectroscopy, for example Ibach [1-3] have reported experimental investigation of ISSE on ZnO surfaces. Theoretically, Lucas and Sunjic [4] explained remarkably well the above quoted experiments by a classical theory which predicted a Poisson distribution of the scattered intensities. Subsequently, Evans and Mills [5,6] gave a quantum-mechanical theory of ISSE based on a Green functions formalism.

The aim of this paper is to present an alternative quantum-mechanical theory of ISSE which predicts all the necessary features of the scattered intensity. We shall use the half space model here, and in the next paper [7] we shall consider a thin film configuration. When a theory is concerned with surface effects, there are many important new features which require that a formalism used in scattering in media of infinite extent must be modified. For example, in the case of ISSE, the incident electrons must enter through the sample boundary before they are scattered, and secondly, the scattered electrons must emerge through the sample boundary before they are detected. These two requirements imply that transmission factors T_I and T_S for the incident and scattered electrons, respectively, must appear in the expressions for the scattering cross-section. These effects appear logically in our formalism.

The plan of this paper is as follows. In Sec.II we describe ISSE as involving three stages, and as we shall see, it is necessary to solve the inhomogeneous Schrödinger equation in order to obtain the scattered wave functions. Sec.III will be devoted to the derivation of the scattering cross-section and our results will be discussed in Sec.IV.

II. SCATTERING GEOMETRY AND WAVE FUNCTIONS

Consider electrons of energy E in region 1 $(z > 0)$ incident into a crystal in region 2 $(z < 0$, and potential $V_0)$. The scattering process can be visualized as broken into three stages illustrated in Fig.1. In the first stage (Fig.1a) an incident electron of wave function ψ_{1I} and frequency ω_i is incident on a crystal surface where there is a partially transmitted wave function ψ_{2I} and a reflected wave fucntion ψ_{1R}, and these are related by solving the homogeneous Schrödinger equation with elementary quantum mechanics

$$\psi_{1R} = R\psi_{1I} \quad . \tag{1a}$$

$$\psi_{2I} = T_I\psi_{1I} \quad , \tag{1b}$$

where

$$R = \frac{k_{1z} - k_{2z}}{k_{1z} + k_{2z}} \quad , \tag{2}$$

$$T_I = \frac{2k_{1z}}{k_{1z} + k_{2z}} \tag{3}$$

and the wavevectors k_{1z} and k_{2z} are given by

$$k_{1z}{}^2 = \frac{2mE}{\hbar^2} - k_{\parallel}{}^2 \quad . \tag{4a}$$

$$k_{2z}{}^2 = \frac{2m}{\hbar^2}(E - V_0) - k_{\parallel}{}^2 \quad , \tag{4b}$$

$$k_{\lambda z}{}^2 + k_{\parallel}{}^2 = k_{\lambda}{}^2 \quad ; \quad \lambda=1,2 \quad . \tag{4c}$$

In stage 2 (Fig.1b) the transmitted electron interacts with a crystal surface excitation of the wavevector $\underline{q}$ and frequency ω to produce a potential

$$\phi_0 e^{i(\underline{Q}\cdot\underline{r} - \omega_s t)} + \text{c.c.} \tag{5}$$

where the frequency ω_s and the wavevector $\underline{Q}$ are given by

$$\omega_s = \omega_i - \omega \quad , \tag{6a}$$

$$\underline{Q} = \underline{k}_{2I} - \underline{q} \quad . \tag{6b}$$

In stage 3 (Fig.1c) the scattered wave fucntions ψ_{1s} and ψ_{2s} are produced, satisfying a homogeneous equation in region 1 and an inhomogeneous Schrödinger equation in region 2 as a result of (5).

$$\left[\frac{\partial^z}{\partial z^2} + \gamma_{1z}{}^2\right]\psi_{1s}(z)e^{i(k_{\parallel}x - \omega_s t)} = 0 \quad , \tag{7}$$

$$\left(\frac{\partial^z}{\partial z^2} + \gamma_{2z}{}^2\right)\psi_{2s}(z)e^{i(k_{\parallel}x - \omega_s t)} = P_0(z)e^{i[(k_{\parallel} + Q_{\parallel})x - (\omega + \omega_s)t]} + \text{c.c.} \tag{8}$$

where in (7) and (8),

$$\gamma_{1z}{}^2 = \frac{2m}{\hbar^2}E_s - k_{\parallel}^2 \quad , \tag{9a}$$

$$\gamma_{2z}{}^2 = \frac{2m}{\hbar^2}(E_s - V_0) - k_{\parallel}{}^2 \quad , \tag{9b}$$

$$P_0(z) = \frac{2m}{\hbar^2}e\,\phi_0(z)\,\psi_{2I}(z) \quad . \tag{9c}$$

After solving (7) and (8) and applying the usual boundary conditions at z = 0, we obtain the scattered fields as

$$\psi_{1s}(z) = f_s\left\{\frac{P_0}{Q_z + \gamma_{2z}} + \frac{P_0^*}{Q_2 - \gamma_{2z}}\right\}e^{ik_{1z}^2 z} \tag{10}$$

$$\psi_{2s}(z) = f_s\left\{\frac{P_0}{Q_z+\gamma_{2z}} + \frac{P_0^*}{Q_z-\gamma_{2z}}\right\}e^{i\gamma_{2z}z} + \frac{P_0[e^{i\gamma z} - e^{iQ_z z}]}{[Q_z{}^2 - \gamma_{2z}{}^2]} + P_0^*\frac{[e^{i\gamma z} - e^{-iQ_z z}]}{[Q_z{}^2 - \gamma_{2z}{}^2]} \tag{11}$$

where

$$f_s = \frac{1}{\gamma_{2z} - k_{1z}} \quad , \tag{12}$$

where in (11) the first term in curly brackets is the complementary function and the other terms are the particular integral. It can be noted that the particular integral terms describe scattering due to bulk excitation and will not be considered further, and in fact they vanish at $z = 0$. Surface effects are in the first term only.

III. SCATTERING CROSS-SECTION

The quantities P_0 and P_0^* are equal in magnitude but opposite in sign, and by using (6b) in (10) and (11), we obtain

$$\psi_{1S}(0) = \psi_{2S}(0) = T_S \frac{|P_0|}{(k_{2z}-q_z)^2 - \gamma_{2z}^2} , \qquad (13)$$

where

$$T_S = \frac{2\gamma_{2z}}{k_{1z} - \gamma_{2z}} \qquad (14)$$

and hence the ratio of the scattered to incident electron current densities is

$$\frac{j_S}{j_I} = \frac{v_S}{v_I} \frac{4m^2e^2|T_I|^2|T_S|^2}{\hbar^4} \frac{<|\phi_0(z)|^2>}{|(k_{2z}-q_z)^2 - \gamma_{2z}^2|^2} , \qquad (15)$$

where v_S and v_I are velocities of the scattered and incident electron, respectively. Eq.(15) may be compared to the results of Refs.4 and 5 by semi-classical and Green functions approaches respectively. This equation gives the scattering efficiency associated with one particular surface excitation. The scattering cross-section, σ, is easily obtained by using (15) and the scattering geometry by a procedure fully explained in Ref.12 and we obtain

$$\sigma = \frac{\omega_i}{\omega_s}\left(\frac{mek_{1S}}{\pi\hbar^2}\right)^2 \cos^2\theta_s \, d\Omega \, A\bar{A} |T_I|^2 |T_S|^2 \frac{<|\phi_0(z)|^2>}{|(k_{2z}-q_z)^2 - \gamma_{2z}^2|^2} , \qquad (16)$$

where θ_s is the scattering angle, $d\Omega$ is an element of solid angle, $\bar{A}$ is the surface area and A is the area through which the scattered beam emerges. The differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{\omega_i}{\omega_s}\left(\frac{mek_{1S}}{\pi\hbar^2}\right)^2 \cos^2\theta_s \, A\bar{A} |T_I|^2 |T_S|^2 \frac{<|\phi_0(z)|^2>}{|(k_{2z}-q_z)^2 - \gamma_{2z}^2|^2} . \qquad (17)$$

The fluctuations in $\langle|\phi_0(z)|^2\rangle$ can be calculated by image-charge techniques on the correspondence principle [13] or response functions theory [12]. In the last referred method, one uses

$$E = -\nabla\phi \qquad (18)$$

and then evaluate electric field fluctuations via the fluctuation-dissipation theorem

$$\langle E_{0i} E_{0j}^* \rangle_\omega = \frac{i\hbar}{2\pi} [n(\omega) + 1][S_{ji}^* - S_{ij}] \qquad (19)$$

where the response functions S_{ij} for the half space have been calculated in Ref.12 and they peak at frequencies of surface excitations given by

$$\epsilon(\omega) = -1 . \qquad (20)$$

IV. DISCUSSION

In this paper we have discussed ISSE by surface excitations by solving the inhomogeneous Schrödinger equation for a crystal in the half space. The main result of our work is Eq.(17). This result correctly depends on factors T_I and T_S that account for transmission of electrons across the boundary as they enter and leave the crystal. The result is general, in the sense that a particular surface excitation depends on $\epsilon(\omega)$ which will affect

$\langle|\phi_0(z)|^2\rangle$ and Mills (5) has discussed such calculations for ionic and non-ionic crystals using image-charge techniques. We have pointed out that alternative calculations are possible through response functions and fluctuation dissipation theorem [12].

A comment needs to be made on the form of the scattered wave function (10) and surface part of (11) where the first terms are inversely proportional to the sum of wave vectors. This denominator is *large*, and hence the back-scattering intensity is small. It is probable that this could be one of the causes why ISSE by *surface* excitations is extremely difficult. This factor has been realized in light scattering experiments (8-12) and one possibility to increase the cross-section is to use forward scattering through a thin film. This has motivated us to repeat our calculation for a thin film configuration, as presented in the next paper [7].

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REFERENCES

[1] H. Ibach, Phys. Rev. Lett. 24, 1416 (1970).

[2] H. Ibach, Phys. Rev. Lett. 27, 253 (1971).

[3] H. Ibach, K. Horn, R. Dorn and H. Lüth, Surf. Sci. 38, 433 (1973).

[4] A.A. Lucas and M. Sunjic, Phys. Rev. Lett. 26, 229 (1971).

[5] E. Evans and D.L. Mills, Phys. Rev. B 5, 4126 (1972).

[6] D.L. Mills, Prog. Surf. Sci. 8, (1977).

[7] J.S. Nkoma, to be published (1982).

[8] A. Denvish and R. Loudon, J. Phys. C 9, L669 (1976).

[9] R. Loudon, J. Phys. (Paris) 26, 677 (1965).

[10] D.R. Tilley, Z. Phys. 254, 71 (1972).

[11] D.L. Mills, A.A. Maradudin and E. Burstein, Ann. Phys. (N.Y.) 56, 504 (1970).

[12] J.S. Nkoma and R. Loudon, J, Phys. C 8, 1950 (1975).

[13] J.S. Nkoma, R. Loudon and D.R. Tilley, J. Phys. C 7, 3547 (1974).

FIGURE CAPTIONS

Fig.1(a) Transmission of the incident electron into the crystal.

Fig.1(b) Interaction of the transmitted electron with a crystal surface excitation.

Fig.1(c) Generation of the scattered electron and its transmission outside the crystal.

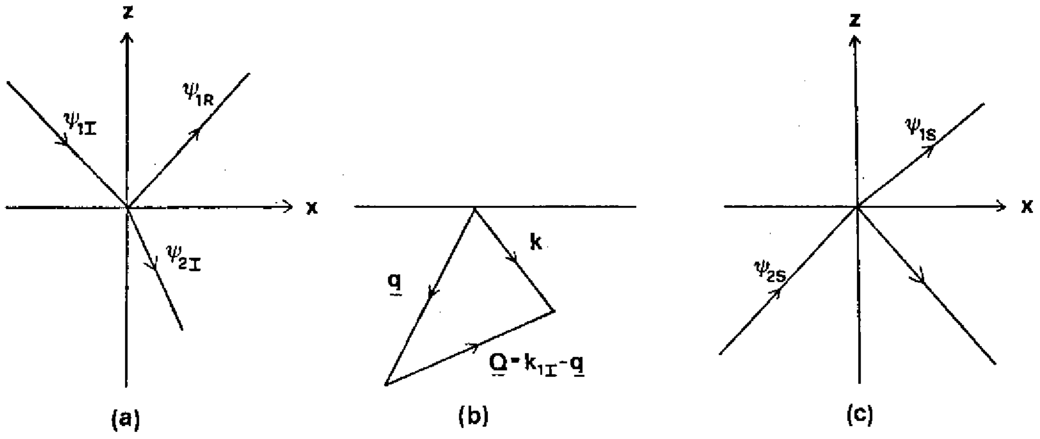

Fig.1

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