

Attenuation of Rayleigh waves by point defects

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A Green's-function method has been used to obtain an expression for the mean free path of a Rayleigh wave propagating along a planar free surface of an isotropic elastic continuum and scattered by a mass defect. The change in density associated with the mass defect is assumed to be $\Delta m \delta(\vec{x}-\vec{x}_0)$, where \vec{x}_0 is the position vector of the defect and Δm is the mass change. The Green's function is evaluated for an isotropic elastic continuum with a stress-free planar surface. Using this Green's function, the continuum equations of motion are formally solved for the particle displacement of the scattered wave in terms of the particle displacement of the incident wave. The Poynting vectors are then calculated for the incident wave and the scattered wave. Explicit results for the scattered-wave Poynting vector are obtained in the asymptotic limit of large distance from the mass defect. The mean free path is then obtained from the ratio of the magnitudes of the incident Poynting vector and the asymptotic scattered Poynting vector. The results are compared with those of other workers.

I. INTRODUCTION

The development of electronic devices using surface elastic waves has stimulated considerable interest in the fundamental properties of these waves. Important among these properties is the rate of scattering of surface waves due to their interaction with various types of defects and with other phonons. The scattering rate can have a significant influence on the performance of devices.

Theoretical investigations of the anharmonic scattering of Rayleigh waves have been carried out by a number of workers. Using a Green's-function procedure, Maradudin and Mills¹ treated the isotropic case using a lattice-dynamical model and found that the damping constant is proportional to $\omega_R T^4$ at low temperatures, where ω_R is the Rayleigh wave frequency and T is the absolute temperature. These results were extended to anisotropic crystals by King and Sheard.² On the experimental side the $\omega_R T^4$ dependence was verified by Salzmann *et al.*³ for several surfaces of quartz.

The effect of defects on the damping of Rayleigh waves was investigated theoretically by Steg and Klemens⁴ for the case of a point-mass defect having a mass change Δm . They used perturbation theory and found that the relaxation rate is proportional to $(\Delta m)^2 \omega_R^5$. Somewhat later, Sakuma^{5,6} reexamined the problem using the Chew-Low scattering formalism and the complete set of normal modes for a semi-infinite isotropic elastic medium constructed by Ezawa.⁷ Sakuma confirmed the ω_R^5 dependence of the scattering rate at sufficiently low frequencies, but in addition, found resonance structure for a defect with a lighter mass than the host atoms. This work has been extended

to the case of random density fluctuations on the surface by Nakayama and Sakuma.⁸

In the present paper the Green's functions for a semi-infinite isotropic elastic continuum with a stress-free planar surface⁹ are used to calculate the inverse attenuation length of a Rayleigh wave scattered by point-mass defects. In Sec. II formal expressions are derived for the amplitude of the scattered wave. In Sec. III these expressions are evaluated explicitly in the asymptotic limit of large distance from the mass defect. In Sec. IV the inverse attenuation length is evaluated. Numerical results are presented in Sec. V. A discussion and comparison with previous work are given in Sec. VI. As we shall see, our results concerning the resonance structure differ significantly from those of Sakuma.

II. SCATTERING OF A RAYLEIGH WAVE BY A MASS DEFECT

In the presence of a mass defect situated at the point $\vec{x}_0 = (0, 0, x_{03})$ in a semi-infinite, isotropic, elastic medium occupying the half space $x_3 > 0$, the equations of motion of the medium can be written in the form

$$-\rho \frac{\partial^2}{\partial t^2} u_\alpha + \sum_{\beta\mu\nu} \frac{\partial C_{\alpha\beta\mu\nu}}{\partial x_\beta} \frac{\partial u_\mu}{\partial x_\nu} + \sum_{\beta\mu\nu} C_{\alpha\beta\mu\nu} \frac{\partial^2 u_\mu}{\partial x_\beta \partial x_\nu} = \rho \sum_\mu L_{\alpha\mu}(\vec{x}, t) u_\mu = \Delta m \delta(\vec{x} - \vec{x}_0) \frac{\partial^2}{\partial t^2} u_\alpha, \quad (2.1)$$

where $u_\alpha(\vec{x}, t)$ is the α Cartesian component of the displacement field at the point \vec{x} at the time t , ρ is the mass density of the medium, and Δm is the increase in the mass of the medium due to the introduction of the defect. In writing Eq. (1) we have assumed that the elastic moduli $\{C_{\alpha\beta\mu\nu}(\vec{x})\}$

are position dependent and are given by

$$C_{\alpha\beta\mu\nu}(\bar{x}) = \Theta(x_3) C_{\alpha\beta\mu\nu}, \quad (2.2)$$

where the $\{C_{\alpha\beta\mu\nu}\}$ are the usual, position-independent elastic moduli of the medium, and $\Theta(x_3)$ is the Heaviside unit step function.

We now introduce a Green's function $G_{\alpha\beta}(\bar{x}, \bar{x}'; t - t')$ as the solution of the equation

$$\sum_{\mu} L_{\alpha\mu}(\bar{x}, t) G_{\mu\beta}(\bar{x}, \bar{x}'; t - t') = \delta_{\alpha\beta} \delta(\bar{x} - \bar{x}') \delta(t - t'), \quad (2.3)$$

subject to outgoing wave or exponentially decaying wave conditions as $x_3 \rightarrow \infty$. In terms of this function we can rewrite Eq. (2.1) as an integral equation.

$$\begin{aligned} u_{\alpha}(\bar{x}, t) = & u_{\alpha}^{(0)}(\bar{x}, t) + \frac{\Delta m}{\rho} \sum_{\beta} \int d^3x' \\ & \times \int dt' G_{\alpha\beta}(\bar{x}, \bar{x}'; t - t') \\ & \times \delta(\bar{x}' - \bar{x}_0) \frac{\partial^2}{\partial t'^2} u_{\beta}(\bar{x}', t'), \end{aligned} \quad (2.4)$$

where $u^{(0)}(\bar{x}, t)$ is a solution of the corresponding homogeneous equation,

$$\sum_{\mu} L_{\alpha\mu}(\bar{x}, t) u_{\mu}^{(0)}(\bar{x}, t) = 0, \quad (2.5)$$

and in the present context represents a Rayleigh wave propagating along the surface $x_3 = 0$ of the semi-infinite elastic medium.

With the Fourier decompositions

$$u_{\alpha}(\bar{x}, t) = u_{\alpha}(\bar{x}, \omega) e^{-i\omega t}, \quad (2.6)$$

$$u_{\alpha}^{(0)}(\bar{x}, t) = u_{\alpha}^{(0)}(\bar{x}, \omega) e^{-i\omega t},$$

$$G_{\alpha\beta}(\bar{x}, \bar{x}'; t - t') = \int \frac{d\Omega}{2\pi} G_{\alpha\beta}(\bar{x}, \bar{x}'; \Omega) e^{-i\Omega(t-t')}, \quad (2.7)$$

$$G_{\alpha\beta}(\bar{x}, \bar{x}'; \Omega) = \int \frac{d^2 k_{\parallel}}{(2\pi)^2} e^{i\bar{k}_{\parallel} \cdot (\bar{x}_{\parallel} - \bar{x}'_{\parallel})} g_{\alpha\beta}(\bar{k}_{\parallel}, \Omega | x_3 x'_3), \quad (2.8)$$

where $\bar{x}_{\parallel} = (x_1, x_2, 0)$ and $\bar{k}_{\parallel} = (k_1, k_2, 0)$, we can rewrite Eq. (2.4) as

$$\begin{aligned} u_{\alpha}(\bar{x}, \omega) = & u_{\alpha}^{(0)}(\bar{x}, \omega) \\ & - \frac{\Delta m \omega^2}{\rho} \sum_{\beta} G_{\alpha\beta}(\bar{x}, \bar{x}_0; \omega) u_{\beta}(\bar{x}_0, \omega). \end{aligned} \quad (2.9)$$

To solve Eq. (2.9) we set $\bar{x} = \bar{x}_0$ and use the fact,

established in the Appendix, that $G_{\alpha\beta}(\bar{x}_0, \bar{x}_0; \omega)$ is a diagonal matrix. In this way we obtain the equation

$$\begin{aligned} u_{\alpha}(\bar{x}_0, \omega) = & u_{\alpha}^{(0)}(\bar{x}_0, \omega) \\ & - \frac{\Delta m \omega^2}{\rho} G_{\alpha\alpha}(\bar{x}_0, \bar{x}_0; \omega) u_{\alpha}(\bar{x}_0, \omega) \end{aligned} \quad (2.10)$$

with the solution

$$u_{\alpha}(\bar{x}_0, \omega) = \frac{u_{\alpha}^{(0)}(\bar{x}_0, \omega)}{1 + (\Delta m \omega^2 / \rho) G_{\alpha\alpha}(\bar{x}_0, \bar{x}_0; \omega)}. \quad (2.11)$$

When we substitute this result into the right-hand side of Eq. (2.9), we find that the amplitude of the scattered displacement field is given by

$$\begin{aligned} u_{\alpha}^{(s)}(\bar{x}, \omega) = & u_{\alpha}(\bar{x}, \omega) - u_{\alpha}^{(0)}(\bar{x}, \omega) \\ = & - \frac{\Delta m \omega^2}{\rho} \sum_{\beta\gamma} G_{\alpha\beta}(\bar{x}, \bar{x}_0; \omega) T_{\beta\gamma}(\bar{x}_0, \omega) \\ & \times u_{\gamma}^{(0)}(\bar{x}_0, \omega), \end{aligned} \quad (2.12)$$

where the scattering matrix is given by

$$\begin{aligned} T_{\alpha\beta}(\bar{x}_0, \omega) = & \frac{\delta_{\alpha\beta}}{1 + (\Delta m \omega^2 / \rho) G_{\alpha\alpha}(\bar{x}_0, \bar{x}_0; \omega)} \\ = & \frac{\delta_{\alpha\beta}}{D_{\alpha}(\bar{x}_0; \omega)}. \end{aligned} \quad (2.13)$$

For the system under consideration it is also the case that the nonzero elements of this matrix obey the relations $T_{11}(\bar{x}_0, \omega) = T_{22}(\bar{x}_0, \omega) \neq T_{33}(\bar{x}_0, \omega)$. With the aid of Eq. (2.8), the scattered field takes the form

$$\begin{aligned} u_{\alpha}^{(s)}(\bar{x}, \omega) = & - \frac{\Delta m \omega^2}{4\pi^2 \rho} \int d^2 k_{\parallel} e^{i\bar{k}_{\parallel} \cdot \bar{x}_{\parallel}} \\ & \times \sum_{\beta} \frac{g_{\alpha\beta}(\bar{k}_{\parallel}, \omega | x_3 x'_3)}{D_{\beta}(\bar{x}_0; \omega)} u_{\beta}^{(0)}(\bar{x}_0, \omega). \end{aligned} \quad (2.14)$$

The Fourier coefficients $\{g_{\alpha\beta}(\bar{k}_{\parallel}, \omega | x_3 x'_3)\}$ can be expressed in terms of another set of coefficients $\{d_{\alpha\beta}(k_{\parallel}, \omega | x_3 x'_3)\}$ by

$$\begin{aligned} g_{\alpha\beta}(\bar{k}_{\parallel}, \omega | x_3 x'_3) = & \sum_{\mu\nu} d_{\mu\nu}(k_{\parallel}, \omega | x_3 x'_3) \\ & \times S_{\mu\alpha}(\hat{k}_{\parallel}) S_{\nu\beta}(\hat{k}_{\parallel}), \end{aligned} \quad (2.15)$$

where the real, orthogonal matrix $\tilde{S}(\hat{k}_{\parallel})$ is given by

$$\tilde{S}(\hat{k}_{\parallel}) = \begin{pmatrix} \hat{k}_1 & \hat{k}_1 & 0 \\ -\hat{k}_2 & \hat{k}_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2.16)$$

The nonzero elements of the tensor $d_{\alpha\beta}(k_{\parallel}, \omega | x_3 x'_3)$, viz. $d_{11}, d_{13}, d_{22}, d_{31}, d_{33}$ have been calculated recently for a semi-infinite, isotropic, elastic medium occupying the upper half space $x_3 > 0$.⁹ Consequently, all of the functions entering the right-hand side

of Eq. (2.14) are known, and the scattered field can thus be calculated. We will return to this aspect of the problem below.

For the incident wave we assume a Rayleigh wave propagating in the positive x_1 direction. If we write the amplitude $u_\alpha^{(0)}(\vec{x}, \omega)$ in the form

$$u_\alpha^{(0)}(\vec{x}, \omega) = u_\alpha^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_3) e^{i\vec{k}_\parallel^{(0)} \cdot \vec{x}_\parallel}, \quad (2.17)$$

with $\vec{k}_\parallel^{(0)} = (k^{(0)}, 0, 0)$, the amplitudes $u_\alpha^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_3)$ are found to be

$$u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_3) = A(e^{-\beta x_3} - \sigma e^{-\beta_t x_3}), \quad (2.18a)$$

$$u_2^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_3) = 0, \quad (2.18b)$$

$$u_3^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_3) = i\rho_1 A[e^{-\beta x_3} - (1/\sigma)e^{-\beta_t x_3}], \quad (2.18c)$$

where A is an arbitrary amplitude. The remaining quantities in Eqs. (2.18) are expressed in terms of c_t and c_t , the speeds of longitudinal and transverse waves in the isotropic elastic medium, respectively, and c_R is the speed of Rayleigh waves. This is obtained from the equation

$$\rho_1^2 \rho_t^2 = \sigma^4, \quad (2.19)$$

with $\sigma = 1 - c_R^2/2c_t^2$, $\rho_t = (1 - c_R^2/c_t^2)^{1/2}$, and $\rho_l = (1 - c_R^2/c_l^2)^{1/2}$. The other quantities entering Eq. (2.18) are defined by

$$\omega = c_R k^{(0)}, \quad \beta_l = k^{(0)} \rho_l, \quad \beta_t = k^{(0)} \rho_t. \quad (2.20)$$

The results expressed by Eqs. (2.17) and (2.18) have the consequence that

$$u_\alpha^{(s)}(\vec{x}, \omega) = -\frac{\Delta m \omega^2}{4\pi^2 \rho} \frac{u_1^{(0)}(k_\parallel^{(0)} \omega | x_{03})}{D_1(\vec{x}_0; \omega)} I_\alpha^{(1)}(\vec{x}; x_{03} | \omega) - \frac{\Delta m \omega^2}{4\pi^2 \rho} \frac{u_3^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_3(\vec{x}_0; \omega)} I_\alpha^{(3)}(\vec{x}; x_{03} | \omega), \quad (2.21)$$

where

$$I_\alpha^{(s)}(\vec{x}; x_{03} | \omega) = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} g_{\alpha\beta}(\vec{k}_\parallel \omega | x_3 x_{03}). \quad (2.22)$$

The resonance denominators $D_\alpha(\vec{x}_0; \omega)$ are evaluated in the Appendix, so that it is only with the integrals $I_\alpha^{(s)}(\vec{x}; x_{03} | \omega)$ that we will be concerned with in what follows.

III. SCATTERED DISPLACEMENT FIELD

In this section we obtain the asymptotic behavior of the integrals $I_\alpha^{(s)}(\vec{x}; x_{03} | \omega)$ defined by Eq. (2.22), for \vec{x} far from the point $(0, 0, x_{03})$. In Sec. IV these results will be used to obtain the elastic Poynting vector of the scattered displacement field, and from the latter the attenuation length of Rayleigh waves due to scattering by mass defects.

Since the results of this section are central to the calculations in the rest of this paper, we pre-

sent their derivation in some detail.

We begin by substituting Eq. (2.15) into Eq. (2.22):

$$I_\alpha^{(s)}(\vec{x}; x_{03} | \omega) = \sum_{\mu\nu} \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} d_{\mu\nu}(k_\parallel \omega | x_3 x_{03}) \times S_{\mu\alpha}(\hat{k}_\parallel) S_{\nu\beta}(\hat{k}_\parallel). \quad (3.1)$$

When the explicit expressions for the matrix elements $\{S_{\alpha\beta}(\hat{k}_\parallel)\}$ are employed in Eq. (3.1), the six integrals $I_\alpha^{(s)}(\vec{x}; x_{03} | \omega)$ which are required for the determination of the scattered wave are given by

$$I_1^{(1)}(\vec{x}; x_{03} | \omega) = I_1 + I_2, \quad (3.2a)$$

$$I_2^{(1)}(\vec{x}; x_{03} | \omega) = I_4 - I_5, \quad (3.2b)$$

$$I_3^{(1)}(\vec{x}; x_{03} | \omega) = I_7, \quad (3.2c)$$

$$I_3^{(1)}(\vec{x}; x_{03} | \omega) = I_3, \quad (3.2d)$$

$$I_2^{(3)}(\vec{x}; x_{03} | \omega) = I_6, \quad (3.2e)$$

$$I_3^{(3)}(\vec{x}; x | \omega) = I_8, \quad (3.2f)$$

where the simpler, auxiliary integrals I_1, \dots, I_8 are defined by

$$I_1 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \cos^2 \varphi d_{11}(k_\parallel \omega | x_3 x_{03}), \quad (3.3a)$$

$$I_2 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \sin^2 \varphi d_{22}(k_\parallel \omega | x_3 x_{03}), \quad (3.3b)$$

$$I_3 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \cos \varphi d_{13}(k_\parallel \omega | x_3 x_{03}), \quad (3.3c)$$

$$I_4 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \cos \varphi \sin \varphi d_{11}(k_\parallel \omega | x_3 x_{03}), \quad (3.3d)$$

$$I_5 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \cos \varphi \sin \varphi d_{22}(k_\parallel \omega | x_3 x_{03}), \quad (3.3e)$$

$$I_6 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \sin \varphi d_{13}(k_\parallel \omega | x_3 x_{03}), \quad (3.3f)$$

$$I_7 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} \cos \varphi d_{31}(k_\parallel \omega | x_3 x_{03}), \quad (3.3g)$$

$$I_8 = \int d^2 k_\parallel e^{i\vec{k}_\parallel \cdot \vec{x}_\parallel} d_{33}(k_\parallel \omega | x_3 x_{03}). \quad (3.3h)$$

Next we represent the vector \vec{x}_\parallel as

$$\vec{x}_\parallel = x_\parallel (\cos \varphi_s, \sin \varphi_s, 0) \quad (3.4)$$

and evaluate the integrals over φ in Eq. (3.3) in the limit of large x_\parallel by the method of stationary phase. The results are

$$I_1 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \cos^2 \varphi_s J_{11}, \quad (3.5a)$$

$$I_2 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \sin^2 \varphi_s J_{22}, \quad (3.5b)$$

$$I_3 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \cos \varphi_s J_{13}, \quad (3.5c)$$

$$I_4 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \sin \varphi_s \cos \varphi_s J_{11}, \quad (3.5d)$$

$$I_5 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \sin \varphi_s \cos \varphi_s J_{22}, \quad (3.5e)$$

$$I_6 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \sin \varphi_s J_{13}, \quad (3.5f)$$

$$I_7 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} \cos \varphi_s J_{31}, \quad (3.5g)$$

$$I_8 \sim \left(\frac{2\pi}{x_{11}}\right)^{1/2} e^{-i\pi/4} J_{33}, \quad (3.5h)$$

where

$$J_{\alpha\beta}(\vec{x}; x_{03} | \omega) = \int_0^\infty dk k^{1/2} e^{ikx_{11}} d_{\alpha\beta}(k\omega | x_3 x_{03}). \quad (3.6)$$

In what follows we focus our attention on the integrals $J_{\alpha\beta}(\vec{x}; x_{03} | \omega)$.

The simplest of these is J_{22} , and its evaluation illustrates many of the ideas to be used in the evaluation of the remaining integrals. From the results of Ref. 9 we have that

$$J_{22}(\vec{x}; x_{03} | \omega) = -\frac{1}{2c_t^2} \int_0^\infty dk \frac{k^{1/2}}{\alpha_t} e^{ikx_{11}} \times (e^{-\alpha_t |x_3 - x_{03}|} + e^{-\alpha_t (x_3 + x_{03})}), \quad (3.7)$$

where

$$\alpha_t = (k^2 - \omega^2/c_t^2)^{1/2}. \quad (3.8)$$

The correct analytical continuation of α_t from the region with $k > \omega/c_t$ to the region $k < \omega/c_t$ is achieved by taking the branch cut along the negative real axis, and assuming ω to have an infinitesimal, positive imaginary part.

Each of the two integrals in Eq. (3.7) is of the form

$$A = \int_0^\infty dk \frac{k^{1/2}}{\alpha_t} e^{f(k)}, \quad (3.9)$$

where

$$f(k) = ikx_{11} - R(k^2 - \omega^2/c_t^2)^{1/2}, \quad (3.10)$$

with R either $|x_3 - x_{03}|$ or $(x_3 + x_{03})$. We expand $f(k)$ about its stationary point k_0 ,

$$f(k) = f(k_0) + \frac{1}{2}(k - k_0)^2 f''(k_0) + \dots, \quad (3.11a)$$

where

$$k_0 = \frac{\omega}{c_t} \frac{x_{11}}{(x_{11}^2 + R^2)^{1/2}}, \quad (3.11b)$$

$$f(k_0) = i \frac{\omega}{c_t} (x_{11}^2 + R^2)^{1/2}, \quad (3.11c)$$

$$f''(k_0) = \frac{c_t}{i\omega} \frac{(x_{11}^2 + R^2)^{3/2}}{R^2}. \quad (3.11d)$$

Since k_0 is in the interval $(0, \infty)$ [in fact, it is in the interval $(0, \omega/c_t)$], we can replace the integration interval $(0, \infty)$ by the infinite interval $(-\infty, \infty)$, in the limit of large x_{11} and x_3 , with an error which is of higher order than the terms we retain. In this way we obtain

$$A \sim \left(\frac{k^{1/2}}{\alpha_t}\right)_{k_0} \exp\left(i \frac{\omega}{c_t} (x_{11}^2 + R^2)^{1/2}\right) \times \int_{-\infty}^{\infty} dk \exp\left(-\frac{i}{2} \frac{c_t}{\omega} \frac{(x_{11}^2 + R^2)^{3/2} k^2}{R^2}\right) = i \frac{(2\pi x_{11})^{1/2}}{(x_{11}^2 + R^2)^{1/2}} e^{-i\pi/4} \exp\left(i \frac{\omega}{c_t} (x_{11}^2 + R^2)^{1/2}\right). \quad (3.12)$$

We now make the assumption that x_{03} is small in comparison with $x = (x_{11}^2 + x_3^2)^{1/2}$. The two values of $(x_{11}^2 + R^2)^{1/2}$ can therefore be expanded in powers of x_{03}/x with the result that

$$(x_{11}^2 + R^2)^{1/2} = x \pm (x_3/x)x_{03} + \frac{1}{2}(x_{11}^2/x^3)x_{03}^2 + \dots, \quad (3.13)$$

where the upper (lower) sign obtains when $R = (x_3 + x_{03})$ ($R = |x_3 - x_{03}|$). We will retain the term linear in x_{03} in the exponential factor in Eq. (3.12), but only the term of zero order in x_{03} in the denominator of the prefactor. The justification for this assumption, which it should be emphasized is convenient but not essential, is the following. In the expressions (2.21) for the amplitudes of the scattered displacement field, the integrals $I_{\alpha}^{(\beta)}(\vec{x}; x_{03} | \omega)$ appear multiplied by the amplitude $u_{\beta}^{(0)}(\vec{k}_{11}^{(0)} | \omega | x_{03})$ of the incident Rayleigh wave at the impurity site. From Eqs. (2.18) we see that these latter amplitudes decay exponentially with increasing x_{03} , so that it is only for $x_{03} \lesssim \beta_t^{-1}$, where β_t ($< \beta_l$) is defined by Eq. (2.20), that any significant scattering of the incident Rayleigh wave by a mass defect can occur. In evaluating the scattered field far from the impurity site, we assume that $k_0 x \gg 1$, where k_0 is the wave vector of the incident Rayleigh wave and is comparable to the wave vectors of the scattered waves, as we will see. If $k_0 x \gg 1$ and $x_{03} \lesssim \beta_t^{-1}$, it follows that $x_{03} \ll x$, and the approximations we are making should lead to little error in the scattered displacement field. To

this approximation we obtain finally for the integral $J_{22}(\vec{x}; x_{03} | \omega)$ the result that

$$J_{22}(\vec{x}; x_{03} | \omega) \sim -\frac{i}{c_t^2} \frac{(2\pi x_{11})^{1/2}}{x} e^{-i\pi/4} e^{i(\omega/c_t)x} \times \cos\left(\frac{\omega}{c_t} \frac{x_3}{x} x_{03}\right). \quad (3.14)$$

It follows, therefore, that the integrals I_2 and I_5 are given asymptotically by

$$I_2 \sim -\frac{2\pi}{c_t^2} \sin^2 \varphi_s \frac{e^{ik_t x}}{x} \cos(k_t x_{03} \cos \theta_s), \quad (3.15a)$$

$$I_5 \sim -\frac{2\pi}{c_t^2} \sin \varphi_s \cos \varphi_s \frac{e^{ik_t x}}{x} \cos(k_t x_{03} \cos \theta_s), \quad (3.15b)$$

where we have used the fact that

$$x_{11} = x \sin \theta_s, \quad x_3 = x \cos \theta_s \quad (3.16)$$

and have defined

$$k_t = \omega/c_t. \quad (3.17)$$

We now turn to the remaining integrals

$J_{\alpha\beta}(\vec{x}; x_{03} | \omega)$ with $\alpha, \beta = 1, 3$. The Green's function $d_{\alpha\beta}(k\omega | x_3 x_{03})$ for $\alpha, \beta = 1, 3$ can be written as⁹

$$d_{\alpha\beta}(k\omega | x_3 x_{03}) = d_{\alpha\beta}^{(1)}(k\omega) e^{-\alpha |x_3 - x_{03}|} + \frac{e^{-\alpha_+ x_3}}{r_+} [d_{\alpha\beta}^{(3)}(k\omega) e^{-\alpha_+ x_{03}} + d_{\alpha\beta}^{(4)}(k\omega) e^{-\alpha_+ x_{03}}] \\ + d_{\alpha\beta}^{(2)}(k\omega) e^{-\alpha_+ |x_3 - x_{03}|} + \frac{e^{-\alpha_+ x_3}}{r_+} [d_{\alpha\beta}^{(5)}(k\omega) e^{-\alpha_+ x_{03}} + d_{\alpha\beta}^{(6)}(k\omega) e^{-\alpha_+ x_{03}}] \quad (3.18)$$

where α_+ has been defined in Eq. (3.8), while

$$\alpha_+ = (k^2 - \omega^2/c_t^2)^{1/2} \quad (3.19)$$

and

$$r_{\pm} = \frac{4\alpha_+ \alpha_+ c_t^2 k^2 \pm (\omega^2 - 2c_t^2 k^2)(\alpha_+^2 + k^2)}{4\alpha_+ \alpha_+ (\omega^2 - 2c_t^2 k^2)}. \quad (3.20)$$

We have factored out the coefficient r_+^{-1} explicitly in Eq. (3.18), because r_+^{-1} has a simple pole at $k = k_R = (\omega + i0)/c_R$, where $c_R (< c_t)$ is the speed of Rayleigh surface waves. Explicit expressions for the coefficient functions $d_{\alpha\beta}^{(i)}(k\omega)$, $i = 1, 2, \dots, 6$ are given in Table I.

The asymptotic forms of the two integrals containing $d_{\alpha\beta}^{(1)}(k\omega)$ and $d_{\alpha\beta}^{(2)}(k\omega)$ can be obtained immediately with the aid of the results we have already obtained. In the former case it is necessary only to replace c_t by c_l in the preceding analysis. Thus we obtain immediately that the integral

$$J_{\alpha\beta}^{(1)}(\vec{x}; x_{03} | \omega) \equiv \int_0^\infty dk k^{1/2} e^{ikx_{11}} d_{\alpha\beta}^{(1)}(k\omega) e^{-\alpha_+ |x_3 - x_{03}|} \quad (3.21a)$$

with $(\alpha, \beta = 1, 3)$ is given asymptotically by

$$J_{\alpha\beta}^{(1)}(\vec{x}; x_{03} | \omega) \sim \frac{1}{i} \frac{(2\pi x_{11})^{1/2}}{2c_t^2} e^{-i\pi/4} \frac{e^{ik_t x} e^{-ik_t x_{03} \cos \theta_s}}{x} \times \begin{pmatrix} \sin^2 \theta_s & \sin \theta_s \cos \theta_s \\ \sin \theta_s \cos \theta_s & \cos^2 \theta_s \end{pmatrix} \quad (3.21b)$$

where

$$k_l = \omega/c_l. \quad (3.22)$$

In a similar fashion we find that the integral

$$J_{\alpha\beta}^{(2)}(\vec{x}; x_{03} | \omega) \equiv \int_0^\infty dk k^{1/2} e^{ikx_{11}} d_{\alpha\beta}^{(2)}(k\omega) e^{-\alpha_+ |x_3 - x_{03}|} \quad (3.23a)$$

is given asymptotically by

$$J_{\alpha\beta}^{(2)}(\vec{x}; x_{03} | \omega) \sim \frac{1}{i} \frac{(2\pi x_{11})^{1/2}}{2c_t^2} e^{-i\pi/4} \frac{e^{ik_t x}}{x} e^{-ik_t x_{03} \cos \theta_s} \times \begin{pmatrix} \cos^2 \theta_s & -\sin \theta_s \cos \theta_s \\ -\sin \theta_s \cos \theta_s & \sin^2 \theta_s \end{pmatrix}. \quad (3.23b)$$

We turn now to the integrals which contain the factor r_+^{-1} in their integrands. We will work out

TABLE I. Coefficient functions $d_{\alpha\beta}^{(i)}(k\omega)$ appearing in Eq. (3.18). The factor ϵ is $\epsilon = \alpha_+ \alpha_+ / k^2$.

$d_{11}^{(1)} = d_{11}^{(4)} = d_{11}^{(5)} = -\frac{k^2}{2\alpha_+ \omega^2}$
$d_{11}^{(2)} = \frac{\epsilon k^2}{2\alpha_+ \omega^2}$
$d_{11}^{(3)} = (1/\epsilon) d_{11}^{(6)} = -\frac{k^2 r_-}{2\alpha_+ \omega^2}$
$d_{13}^{(1)} = -d_{13}^{(2)} = d_{31}^{(1)} = -d_{31}^{(2)} = -\frac{ik}{2\omega^2} \operatorname{sgn}(x_3 - x_{03})$
$d_{13}^{(3)} = d_{13}^{(6)} = -d_{31}^{(3)} = -d_{31}^{(6)} = \frac{ikr_-}{2\omega^2}$
$d_{13}^{(4)} = -d_{31}^{(5)} = \frac{ik}{2\omega^2} \frac{1}{\epsilon}$
$d_{13}^{(5)} = -d_{31}^{(4)} = \frac{ik}{2\omega^2}$
$d_{33}^{(1)} = \frac{\epsilon k^2}{2\alpha_+ \omega^2}$
$d_{33}^{(2)} = d_{33}^{(3)} = d_{33}^{(6)} = -\frac{k^2}{2\alpha_+ \omega^2}$
$d_{33}^{(4)} = \epsilon d_{33}^{(6)} = -\frac{\epsilon k^2 r_-}{2\alpha_+ \omega^2}$

one of them explicitly, and will simply quote the results for the remaining three. The integral we consider is

$$J_{\alpha\beta}^{(3)}(\vec{x}; x_{03} | \omega) = \int_0^\infty dk e^{ikx_{11} - \alpha i x_3} \frac{k^{1/2}}{r_+} d_{\alpha\beta}^{(3)}(k\omega) e^{-\alpha i x_{03}}. \tag{3.24}$$

To evaluate this integral in the limit of large x we divide the range of integration $(0, \infty)$ into two parts: $(0, \omega/c_l)$ and $(\omega/c_l, \infty)$, and consider the resulting two integrals separately.

A. Contribution from the interval $(0, \omega/c_l)$

We evaluate the integral

$$J_{\alpha\beta}^{(3a)}(\vec{x}; x_{03} | \omega) = \int_0^{\omega/c_l} dk e^{ikx_{11} - \alpha i x_3} \frac{k^{1/2}}{r_+} \times d_{\alpha\beta}^{(3)}(k\omega) e^{-\alpha i x_{03}} \tag{3.25}$$

$$J_{\alpha\beta}^{(3a)}(\vec{x}; x_{03} | \omega) \sim \left(\frac{k^{1/2}}{r_+} d_{\alpha\beta}^{(3)}(k\omega) e^{-\alpha i x_{03}} \right) k_0 e^{ik_1 x} \int_{-\infty}^{\infty} dk \exp\left(-\frac{i}{2} \frac{c_l}{\omega} \frac{x^3}{x_3^2} k^2\right) \\ = \frac{1}{i} \frac{(2\pi x_{11})^{1/2}}{2c^2} e^{-i\pi/4} \frac{e^{ik_1 x}}{x} e^{ik_1 x_{03} \cos\theta_s} \frac{\omega^2 - 4\lambda^3 v \sin^2\theta_s \cos\theta_s}{\omega^2 + 4\lambda^3 v \sin^2\theta_s \cos\theta_s} \begin{pmatrix} -\sin^2\theta_s & \sin\theta_s \cos\theta_s \\ -\sin\theta_s \cos\theta_s & \cos^2\theta_s \end{pmatrix}, \tag{3.28}$$

where

$$v = (1 - \lambda^2 \sin^2\theta_s)^{1/2}, \quad w = 1 - 2\lambda^2 \sin^2\theta_s, \tag{3.29} \\ \lambda = c_l/c_t < 1.$$

We have used the results of Table I in obtaining this result.

B. Contribution from the interval $(\omega/c_l, \infty)$

To evaluate the contribution to $J_{\alpha\beta}^{(3)}(\vec{x}; x_{03} | \omega)$ from the integration range $\omega/c_l < k < \infty$, we regard k as a complex variable and consider the contour integral

$$J_{\alpha\beta}^{(3b)}(\vec{x}; x_{03} | \omega) = \int_{C_l} dk e^{ikx_{11} - \alpha i x_3} \frac{k^{1/2}}{r_+} \times d_{\alpha\beta}^{(3)}(k\omega) e^{-\alpha i x_{03}}, \tag{3.30}$$

where the contour C_l is shown in Fig. 1. The integrand can be made single valued inside and on this contour by a proper choice of branch cuts. Then by employing the same arguments that were used in Ref. 9 in connection with the evaluation of a similar integral, in the limit as the circular portion of the contour recedes to infinity the integral

$$J_{\alpha\beta}^{(3b)}(\vec{x}; x_{03} | \omega) = \int_{\omega/c_l}^\infty dk e^{ikx_{11} - \alpha i x_3} \frac{k^{1/2}}{r_+} \times d_{\alpha\beta}^{(3)}(k\omega) e^{-\alpha i x_{03}} \tag{3.31}$$

by the method of stationary phase. If we denote by k_0 the stationary point of the function

$$f(k) = ikx_{11} - \left(k^2 - \frac{\omega^2}{c_l^2}\right)^{1/2} x_3 \\ = f(k_0) + \frac{1}{2} f''(k_0)(k - k_0)^2 + \dots, \tag{3.26}$$

we find that

$$k_0 = (\omega/c_l)(x_{11}/x) < \omega/c_l, \tag{3.27a}$$

$$f(k_0) = ik_1 x, \tag{3.27b}$$

$$f''(k_0) = -i(c_l/\omega)(x^3/x_3^2). \tag{3.27c}$$

We therefore obtain for the large- x limit of the integral (3.25)

is given by $2\pi i$ times the residue at the simple pole the integrand possesses at the zero of r_+ at $k = k_R = (\omega + i0)/c_R$. In the vicinity of this pole we have the expansion⁹

$$\frac{1}{r_+} = -\frac{2\omega}{c_R R} \frac{1}{(k - k_R)} + \dots, \tag{3.32a}$$

where the dots stand for analytical terms and

$$R = \frac{1}{\sigma^5} \left[\frac{c_R^4}{c_t^4} \left(1 + 2 \frac{c_t^2}{c_l^2}\right) - \frac{c_R^2}{c_t^2} \left(9 - 5 \frac{c_t^2}{c_l^2}\right) + 8 \left(1 - \frac{c_t^2}{c_l^2}\right) \right]. \tag{3.32b}$$

Consequently, we obtain immediately that

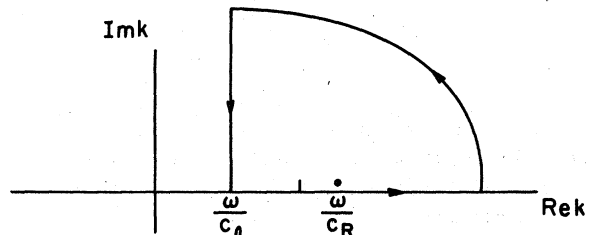


FIG. 1. Contour for the evaluation of the integral in Eq. (3.30).

$$J_{\alpha\beta}^{(3b)}(\vec{x}; x_{03} | \omega) \sim -\frac{\pi i}{2R\omega^2} \left(\frac{\omega}{c_R}\right)^{5/2} e^{ik_R x_{11}} e^{-\beta_l(x_3+x_{03})} \frac{(2\sigma)^2 + 4(\rho_t)(\rho_l)}{(2\sigma)(\rho^2)(\rho_t)} \begin{pmatrix} 1 & -i\rho^l \\ i\rho_t & \rho_t^2 \end{pmatrix}. \quad (3.33)$$

In the same way we obtain the asymptotic behaviors of the remaining integrals. We omit the details and merely present the results. We have that

$$\begin{aligned} J_{\alpha\beta}^{(4)}(\vec{x}; x_{03} | \omega) &= \int_0^\infty dk e^{ikx_{11}} e^{-\alpha_l x_3} \frac{k^{1/2}}{r_+} d_{\alpha\beta}^{(4)}(k\omega) e^{-\alpha_l x_{03}} \\ &\sim \frac{1}{i} \frac{(2\pi x_{11})^{1/2}}{2c_t^2} \cos\theta_s \sin\theta_s e^{-i\tau/4} \frac{e^{ik_t x}}{x} e^{i(\omega/c_t)x_{03}} \frac{4\lambda v \omega \cos\theta_s}{\omega^2 + 4\lambda^3 v \sin^2\theta_s \cos\theta_s} \\ &\quad \times \begin{pmatrix} \tan\theta_s & \lambda \sin^2\theta_s / v \cos\theta_s \\ 1 & \lambda \sin\theta_s / v \end{pmatrix} + \frac{2\pi i}{R\omega^2} \left(\frac{\omega}{c_R}\right)^{5/2} e^{ik_R x_{11}} e^{-\beta_l x_3 - \beta_l x_{03}} \frac{1}{\rho_t \rho_l} \begin{pmatrix} \rho_t & -i \\ i\rho_t \rho_l & \rho_l \end{pmatrix}; \end{aligned} \quad (3.34)$$

$$\begin{aligned} J_{\alpha\beta}^{(5)}(\vec{x}; x_{03} | \omega) &= \int_0^\infty dk e^{ikx_{11}} e^{-\alpha_l x_3} \frac{k^{1/2}}{R_+} d_{\alpha\beta}^{(5)}(k\omega) e^{-\alpha_l x_{03}} \\ &\sim \frac{1}{i} \frac{(2\pi x_{11})^{1/2}}{2c_t^2} \cos\theta_s \sin\theta_s e^{-\tau/4} \frac{e^{ik_t x}}{x} \exp\left(i\epsilon(\theta_s) \frac{\omega}{c_t} x_{03} |\lambda^2 - \sin^2\theta_s|^{1/2}\right) \\ &\quad \times \frac{4\epsilon(\theta_s) \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} (1 - 2\sin^2\theta_s)}{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + (1 - 2\sin^2\theta_s) \cos 2\theta_s} \\ &\quad \times \begin{pmatrix} \sin\theta_s / \epsilon(\theta_s) |\lambda^2 - \sin^2\theta_s|^{1/2} & -1 \\ -\tan\theta_s \sin\theta_s / \epsilon(\theta_s) |\lambda^2 - \sin^2\theta_s|^{1/2} & \tan\theta_s \end{pmatrix} \\ &\quad + \frac{2\pi i}{R\omega^2} \left(\frac{\omega}{c_R}\right)^{5/2} e^{ik_R x_{11}} e^{-\beta_l x_3 - \beta_l x_{03}} (1/\rho_t \rho_l) \begin{pmatrix} \rho_t & -i\rho_t \rho_l \\ i & \rho_l \end{pmatrix}, \end{aligned} \quad (3.35)$$

where we have introduced

$$\epsilon(\theta_s) = \begin{cases} 1, & 0 < \sin\theta_s < \lambda \\ i, & \lambda < \sin\theta_s < 1; \end{cases} \quad (3.36)$$

$$\begin{aligned} J_{\alpha\beta}^{(6)}(\vec{x}; x_{03} | \omega) &= \int_0^\infty dk e^{ikx_{11}} e^{-\alpha_l x_3} \frac{k^{1/2}}{r_+} d_{\alpha\beta}^{(6)}(k\omega) e^{-\alpha_l x_{03}} \\ &\sim \frac{1}{i} \frac{(2\pi x_{11})^{1/2}}{2c_t^2} e^{-i\tau/4} \frac{e^{ik_t x}}{x} e^{i(\omega/c_t)x_{03} \cos\theta_s} \\ &\quad \times \frac{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} - (1 - 2\sin^2\theta_s) \cos 2\theta_s}{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + (1 - 2\sin^2\theta_s) \cos 2\theta_s} \begin{pmatrix} -\cos^2\theta_s & -\sin\theta_s \cos\theta_s \\ \sin\theta_s \cos\theta_s & \sin^2\theta_s \end{pmatrix} \\ &\quad - \frac{\pi i}{2R\omega^2} \left(\frac{\omega}{c_R}\right)^{5/2} e^{ik_R x_{11}} e^{-\beta_l(x_3+x_{03})} \frac{(2\sigma)^2 + 4\rho_t \rho_l}{2\sigma \rho_t \rho_l^2} \begin{pmatrix} \rho_t^2 & -i\rho_t \\ i\rho_t & 1 \end{pmatrix}. \end{aligned} \quad (3.37)$$

The results of this section when substituted into Eq. (2.21) enable us to write the amplitude of the scattered displacement field $\vec{u}^{(s)}(\vec{x}, \omega)$ as the sum of four contributions:

$$\begin{aligned} \vec{u}^{(s)}(\vec{x}, \omega) &= \vec{u}^{(l)}(\vec{x}, \omega) + \vec{u}^{(ts)}(\vec{x}, \omega) \\ &\quad + \vec{u}^{(ts)}(\vec{x}, \omega) + \vec{u}^{(R)}(\vec{x}, \omega). \end{aligned} \quad (3.38)$$

In Eq. (3.38) $\vec{u}^{(l)}(\vec{x}, \omega)$ is the amplitude describing the scattering of the incident Rayleigh wave into bulk longitudinal waves; $\vec{u}^{(ts)}(\vec{x}, \omega)$ [$\vec{u}^{(ts)}(\vec{x}, \omega)$] is the amplitude for scattering into bulk transverse waves of p polarization (s polarization); and $\vec{u}^{(R)}(\vec{x}, \omega)$ is the amplitude for scattering into other Rayleigh waves. The explicit expressions for each

of these amplitudes have the following simple forms.

$$\bar{u}^{(l)}(\bar{x}, \omega) = \frac{\bar{x}}{x} \frac{\Delta m \omega^2}{4\pi\rho c_t^2} u_l \frac{e^{ik_l x}}{x}, \quad (3.39a)$$

$$u_l = \frac{u_1^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_1(\bar{x}_0; \omega)} \sin\theta_s \cos\varphi_s F_1(\theta_s, x_{03}) + \frac{u_3^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_3(\bar{x}_0; \omega)} \cos\theta_s F_2(\theta_s, x_{03}), \quad (3.39b)$$

where

$$F_1(\theta_s, x_{03}) = e^{-ik_l x_{03} \cos\theta_s} - e^{ik_l x_{03} \cos\theta_s} \frac{w^2 - 4\lambda^3 v \sin^2\theta_s \cos\theta_s}{w^2 + 4\lambda^3 v \sin^2\theta_s \cos\theta_s} + e^{ik_l v x_{03}} \frac{4\lambda w v \cos\theta_s}{w^2 + 4\lambda^3 v \sin^2\theta_s \cos\theta_s^{1/2}}; \quad (3.39c)$$

$$F_2(\theta_s, x_{03}) = e^{-ik_l x_{03} \cos\theta_s} + e^{ik_l x_{03} \cos\theta_s} \frac{w^2 - 4\lambda^3 v \sin^2\theta_s \cos\theta_s}{w^2 + 4\lambda^3 v \sin^2\theta_s \cos\theta_s} + e^{ik_l v x_{03}} \frac{4\lambda^2 w \sin^2\theta_s}{w^2 + 4\lambda^3 v \sin^2\theta_s \cos\theta_s}. \quad (3.39d)$$

$$\bar{u}^{(tp)}(\bar{x}, \omega) = \frac{\Delta m \omega^2}{4\pi\rho c_t^2} u_t^{(p)} \frac{e^{ik_t x}}{x} \times (\hat{x}_1 \cos\theta_s \cos\varphi_s + \hat{x}_2 \cos\theta_s \sin\varphi_s - \hat{x}_3 \sin\theta_s), \quad (3.40a)$$

$$u_t^{(p)} = \frac{u_1^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_1(\bar{x}_0; \omega)} \cos\theta_s \cos\varphi_s G_1(\theta_s, x_{03}) - \frac{u_3^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_3(\bar{x}_0; \omega)} \sin\theta_s G_2(\theta_s, x_{03}), \quad (3.40b)$$

where

$$G_1(\theta_s, x_{03}) = e^{-ik_t x_{03} \cos\theta_s} + \exp[i\epsilon(\theta_s) k_t x_{03} |\lambda^2 - \sin^2\theta_s|^{1/2}] \frac{4 \sin^2\theta_s \cos 2\theta_s}{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + \cos^2 2\theta_s} - e^{ik_t x_{03} \cos\theta_s} \frac{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} - \cos^2 2\theta_s}{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + \cos^2 2\theta_s}; \quad (3.40c)$$

$$G_2(\theta_s, x_{03}) = e^{-ik_t x_{03} \cos\theta_s} + \exp[i\epsilon(\theta_s) k_t x_{03} |\lambda^2 - \sin^2\theta_s|^{1/2}] \frac{4\epsilon(\theta_s) \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} \cos 2\theta_s}{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + \cos^2 2\theta_s} + e^{ik_t x_{03} \cos\theta_s} \frac{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} - \cos^2 2\theta_s}{4\epsilon(\theta_s) \sin^2\theta_s \cos\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + \cos^2 2\theta_s}. \quad (3.40d)$$

$$\bar{u}^{(ts)}(\bar{x}, \omega) = \frac{\Delta m \omega^2}{2\pi\rho c_t^2} \frac{e^{ik_t x}}{x} (\hat{x}_1 \sin\varphi_s - \hat{x}_2 \cos\varphi_s) \frac{u_1^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_1(\bar{x}_0; \omega)} \sin\varphi_s \cos(k_t x_{03} \cos\theta_s). \quad (3.41)$$

$$\bar{u}^{(R)}(\bar{x}, \omega) = 2 \frac{c_t^2}{c_R} u_R \frac{e^{ik_R x_{11}}}{x_{11}^{1/2}} \{ (\hat{x}_1 \cos\varphi_s + \hat{x}_2 \sin\varphi_s + \hat{x}_3 i\rho_l) e^{-\beta_l x_3} - \sigma [\hat{x}_1 \cos\varphi_s + \hat{x}_2 \sin\varphi_s + \hat{x}_3 (i/\rho_t)] e^{-\beta_t x_3} \}, \quad (3.42a)$$

$$u_R = \frac{1}{2R} \left(\frac{i}{2\pi} \right)^{1/2} \frac{\Delta m}{\rho} \frac{\omega^{5/2}}{c_R^{1/2} c_t^2} \frac{1}{\rho_l \sigma} \times \left[\cos\varphi_s (e^{-\beta_l x_{03}} - \sigma e^{-\beta_t x_{03}}) \frac{u_1^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_1(\bar{x}_0; \omega)} - i\rho_l \left(e^{-\beta_l x_{03}} - \frac{e^{-\beta_t x_{03}}}{\sigma} \right) \frac{u_3^{(0)}(\bar{k}_{\parallel}^{(0)} \omega | x_{03})}{D_3(\bar{x}_0; \omega)} \right]. \quad (3.42b)$$

We now turn to the determination of the elastic Poynting vector of the scattered displacement field, and from it the inverse attenuation length of a Rayleigh wave in the presence of point defects.

IV. EVALUATION OF THE INVERSE ATTENUATION LENGTH

The first step in the evaluation of the inverse attenuation length is the calculation of the elastic Poynting vector for the incident and scattered waves. In their paper concerning the attenuation of Rayleigh waves by surface roughness, Maradudin and Mills⁹ derive the following expression for the complex Poynting vector $\bar{\zeta}^c$ of an elastic wave propagating in an isotropic medium,

$$\bar{\zeta}^c = (\zeta_1^c, \zeta_2^c, \zeta_3^c), \quad (4.1)$$

where

$$\zeta_1^c = -\frac{1}{2} \rho \dot{u}_1^* \left[c_1^2 (\bar{\nabla} \cdot \bar{u}) - 2c_t^2 \left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) \right] - \frac{1}{2} \rho c_t^2 \left[\dot{u}_2^* \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) + \dot{u}_3^* \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \right], \quad (4.2)$$

and the expressions for ζ_2^c and ζ_3^c can be obtained by cyclic permutation of the subscripts in Eq. (4.2). We shall assume that the displacement components u_α vary with time as $\exp(-i\omega t)$, so that $u_\alpha^* \sim \exp(i\omega t)$ and $\dot{u}_\alpha^* = i\omega u_\alpha^*$. Then Eq. (4.2) can be rewritten as

$$\begin{aligned} \zeta_1^c = & -\frac{1}{2} i \omega \rho u_1^* \left[c_t^2 (\nabla \cdot \vec{u}) - 2c_t^2 \left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) \right. \\ & \left. - \frac{1}{2} i \omega \rho c_t^2 \left[u_2^* \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) + u_3^* \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \right] \right]. \end{aligned} \quad (4.3)$$

We take up first the Poynting vector of the incident Rayleigh wave $\vec{\zeta}^c(i)$. The displacement field for the incident wave is given by Eqs. (2.17) and (2.18). We have taken the direction of propagation to be the 1 direction, so the only component of the Poynting vector of interest is $\zeta_1^c(i)$. The latter is given

$$\begin{aligned} \zeta_1^c(i) = & |A|^2 \frac{\rho c_t^2 \omega^2}{c_R} \\ & \times (\zeta_{11} e^{-2\beta t x_3} + \zeta_{1t} e^{-(\beta t + \beta_t) x_3} + \zeta_{tt} e^{-2\beta t x_3}), \end{aligned} \quad (4.4)$$

where

$$\zeta_{11} = 2 + \frac{c_R^2}{2c_t^2} \left(1 - 4 \frac{c_t^2}{c_i^2} \right), \quad (4.5a)$$

$$\zeta_{1t} = -\sigma \left(2 + \frac{c_R^2}{2c_t^2} - \frac{c_R^2}{c_i^2} \right) - \frac{\rho_i^2 (2 - c_R^2 / 2c_t^2)}{\sigma}, \quad (4.5b)$$

$$\zeta_{tt} = \frac{1}{\sigma} (\sigma^3 + \rho_i^2). \quad (4.5c)$$

We now consider the contributions to the Poynting vector of the scattered wave associated with the different types of waves constituting the latter.

A. Scattering into longitudinal bulk waves

The scattered displacement field is given by Eq. (3.39a). The derivatives with respect to the coordinate components are found to be

$$\frac{\partial u_\alpha^{(l)}(\vec{x}, \omega)}{\partial x_\beta} = \frac{i k_t x_\beta}{x} u_\alpha^{(l)}(\vec{x}, \omega) \quad (4.6)$$

in the limit $x \rightarrow \infty$. Substituting this result into Eq. (4.3), we obtain

$$\begin{aligned} \zeta_1^c(l) = & \frac{1}{2} \frac{\rho \omega^2}{c_l x} u_1^* \left[c_l^2 (\vec{x} \cdot \vec{u}) - 2c_l^2 (x_2 u_2 + x_3 u_3) \right] \\ & + \frac{1}{2} \frac{\rho \omega^2 c_l^2}{c_l x} \left[u_2^* (x_2 u_1 + x_1 u_2) + u_3^* (x_3 u_1 + x_1 u_3) \right]. \end{aligned} \quad (4.7)$$

Again using Eq. (3.39a), we find that this contribution to the Poynting vector can be written in the form

$$\vec{\zeta}^c(l) = (\Delta m)^2 \omega^6 |u_l|^2 \vec{x} / 32\pi^2 \rho c_l^3 x^3. \quad (4.8)$$

B. Scattering into *p*-polarized transverse bulk waves

For this case the derivatives of the scattered displacement field components with respect to the coordinate components can be written as

$$\frac{\partial u_\alpha^{(tp)}(\vec{x}, \omega)}{\partial x_\beta} = \frac{i k_t x_\beta}{x} u_\alpha^{(tp)}(\vec{x}, \omega) \quad (4.9)$$

in the limit $x \rightarrow \infty$. The corresponding contribution to the Poynting vector can then be expressed as

$$\vec{\zeta}^c(tp) = (\Delta m)^2 \omega^6 |u_t^{(p)}|^2 \vec{x} / 32\pi^2 \rho c_t^3 x^3. \quad (4.10)$$

C. Scattering into *s*-polarized transverse bulk waves

In the limit $x \rightarrow \infty$, the expressions for the derivatives of the scattered displacement field components with respect to the coordinate components can be written in a form analogous to Eq. (4.9), namely,

$$\frac{\partial u_\alpha^{(ts)}(\vec{x}, \omega)}{\partial x_\beta} = \frac{i k_t x_\beta}{x} u_\alpha^{(ts)}(\vec{x}, \omega). \quad (4.11)$$

Using Eq. (3.41) we see that the Poynting vector from *s*-polarized transverse bulk waves takes the form

$$\vec{\zeta}^c(ts) = (\Delta m)^2 \omega^6 |u_t^{(s)}|^2 \vec{x} / 8\pi^2 \rho c_t^3 x^3 \quad (4.12)$$

where

$$u_t^{(s)} = \frac{u_1^{(0)}(k_{||}^{(0)} \omega |x_{03}|)}{D_1(\vec{x}_0; \omega)} \sin \varphi_s \cos(k_t x_{03} \cos \theta_s). \quad (4.13)$$

D. Scattering into other Rayleigh waves

The scattered displacement field for this case is given by Eq. (3.42). If we compare this result with that for the incident displacement field given by Eqs. (2.17) and (2.18) and use the Rayleigh wave dispersion relation, Eq. (2.19), we see that the two displacement fields differ only in the replacement

$$A \rightarrow 2(c_t^2/c_R^2)(u_R/x_1^{1/2}) \quad (4.14)$$

and in the direction of propagation parallel to the surface. Consequently, we can obtain the magnitude of the Poynting vector by taking that for the incident Rayleigh wave, Eq. (4.4), and making the replacement specified by Eq. (4.14).

The next step in the calculation of the inverse attenuation length is to evaluate the energy stored per unit time in the incident and scattered waves. For the incident wave, the energy stored per unit time is given by⁹

$$\frac{dE_0}{dt} = L_2 \int_0^\infty dx_3 \zeta_1^c(i), \quad (4.15)$$

where L_2 is the dimension of the sample parallel to the surface and perpendicular to the direction of propagation. Substituting Eq. (4.4) into Eq. (4.15), we obtain

$$\frac{dE_0}{dt} = |A|^2 L_2 \omega^2 \rho \frac{c_t^2}{c_R} \left(\frac{\zeta_{II}}{2\beta_t} + \frac{\zeta_{It}}{(\beta_t + \beta_t)} + \frac{\zeta_{tt}}{2\beta_t} \right). \quad (4.16)$$

Turning now to the energy stored per unit time in the scattered wave, we present results for each type of scattered wave separately. For the longitudinal scattered wave, the energy stored

$$\frac{dE_l}{dt} = \frac{(\Delta m)^2 \omega^6}{32\pi \rho c_t^3} \int_0^{\pi/2} d\theta_s \left(\sin^3 \theta_s \left| \frac{u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_1(\vec{x}_0; \omega)} F_1(\theta_s, x_{03}) \right|^2 + 2 \sin \theta_s \cos^2 \theta_s \left| \frac{u_3^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_3(\vec{x}_0; \omega)} F_2(\theta_s, x_{03}) \right|^2 \right). \quad (4.19)$$

An expression analogous to Eq. (4.17) can be applied to the case of p -polarized transverse scattered waves. Using Eq. (4.10) for the Poynting vector and Eq. (3.40b) for $u_t^{(p)}$, we obtain for the energy stored per unit time

$$\frac{dE_t^{(p)}}{dt} = \frac{(\Delta m)^2 \omega^6}{32\pi \rho c_t^3} \int_0^{\pi/2} d\theta_s \left(\sin \theta_s \cos^2 \theta_s \left| \frac{u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_1(\vec{x}_0; \omega)} G_1(\theta_s, x_{03}) \right|^2 + 2 \sin^3 \theta_s \left| \frac{u_3^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_3(\vec{x}_0; \omega)} G_2(\theta_s, x_{03}) \right|^2 \right). \quad (4.20)$$

For the case of s -polarized transverse scattered waves, we use Eqs. (4.13) and (4.17) and find for the energy stored per unit time

$$\frac{dE_t^{(s)}}{dt} = \frac{(\Delta m)^2 \omega^6}{8\pi \rho c_t^3} \left| \frac{u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_1(\vec{x}_0; \omega)} \right|^2 \frac{\sin k_t x_{03}}{k_t x_{03}}. \quad (4.21)$$

Finally, for the case of scattering into other Rayleigh waves, we can write the energy stored per unit time in the form

$$\frac{dE_R}{dt} = x_\parallel \int_0^\infty dx_3 \int_0^{2\pi} d\varphi_s |\zeta_R^c|. \quad (4.22)$$

Using Eq. (4.4) and the replacement specified by Eq. (4.14), we carry out the integration over x_3 and obtain

$$\frac{dE_R}{dt} = 2\rho\omega\epsilon \frac{c_t^6}{c_R^4} \int_0^{2\pi} d\varphi_s |u_R|^2, \quad (4.23)$$

where

$$\epsilon = \frac{\zeta_{II}}{\rho_t} + \frac{2\zeta_{It}}{\rho_t + \rho_t} + \frac{\zeta_{tt}}{\rho_t}. \quad (4.24)$$

The integration over φ_s can be accomplished with the aid of Eq. (3.42b) to yield the result

$$\begin{aligned} \frac{dE_R}{dt} &= \frac{(\Delta m)^2 \omega^6 c_t^6 \epsilon}{4\rho R^2 c_R^5 \rho_t^2 \sigma^2} \\ &\times \left[(e^{-\beta_t x_{03}} - \sigma e^{-\beta_t x_{03}})^2 \left| \frac{u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_1(\vec{x}_0; \omega)} \right|^2 \right. \\ &\quad \left. + 2\rho_t^2 \left(e^{-\beta_t x_{03}} - \frac{e^{-\beta_t x_{03}}}{\sigma} \right)^2 \left| \frac{u_3^{(0)}(\vec{k}_\parallel^{(0)} \omega | x_{03})}{D_3(\vec{x}_0; \omega)} \right|^2 \right]. \end{aligned} \quad (4.25)$$

per unit time is given by

$$\frac{dE_t}{dt} = \int_0^{\pi/2} d\theta_s \int_0^{2\pi} d\varphi_s |\vec{x}|^2 \sin \theta_s |\zeta^c(t)|. \quad (4.17)$$

Using Eq. (4.8), this result becomes

$$\frac{dE_t}{dt} = \frac{(\Delta m)^2 \omega^6}{32\pi^2 \rho c_t^3} \int_0^{\pi/2} d\theta_s \int_0^{2\pi} d\varphi_s \sin \theta_s |u_t|^2. \quad (4.18)$$

The integration over φ_s can be carried out with the aid of Eq. (3.39b) yielding

We are now in a position to calculate the various contributions to the inverse attenuation lengths. We consider separately the two cases of mass defects localized at the surface $x_3 = 0$ and of mass defects uniformly distributed throughout the crystal.

Turning first to the case of defects localized at the surface, we consider a rectangular patch of surface with dimensions L_1 and L_2 , respectively, parallel and perpendicular to the direction of propagation of the incident surface wave and with n_s defects per unit area. The fraction of the incident energy radiated into longitudinal bulk waves is given by

$$f_l = L_1 L_2 n_s \frac{dE_l}{dt} / \frac{dE_0}{dt}. \quad (4.26)$$

The corresponding contribution to the inverse attenuation length is

$$1/l^{(l)} = f_l / L_1. \quad (4.27)$$

For defects at the surface, $x_{03} = 0$, we find from Eqs. (2.18)

$$|u_3^{(0)}(k_\parallel^{(0)} \omega | 0)|^2 = (\sigma_t^2 / \sigma^2) |u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | 0)|^2, \quad (4.28)$$

$$|u_1^{(0)}(\vec{k}_\parallel^{(0)} \omega | 0)|^2 = (c_R^4 / 4c_t^4) |A|^2. \quad (4.29)$$

If we use these results and set x_{03} equal to zero in Eqs. (3.39c) and (3.39d) for $F_1(\theta_s, x_{03})$ and $F_2(\theta_s, x_{03})$, we can simplify Eq. (4.19) for dE_l/dt and obtain the result

$$\frac{1}{\bar{l}^{(T)}} = \frac{n_s(\Delta m)^2 \omega^5 c_R^4}{4\pi \rho^2 c_i^3 \epsilon} \int_0^{\pi/2} d\theta_s \frac{\sin\theta_s \cos^2\theta_s}{(4\lambda^3 v \cos\theta_s \sin^2\theta_s + w^2)^2} \left(\frac{\lambda^2 v^2 \sin^2\theta_s}{|D_1(0; \omega)|^2} + \frac{\rho_i^2 w^2}{2\sigma^2 |D_3(0; \omega)|^2} \right). \quad (4.30)$$

In a similar fashion, the contribution of p -polarized transverse bulk waves to the inverse attenuation length can be obtained from Eqs. (4.20) and (4.26)–(4.29) with the result

$$\frac{1}{\bar{l}^{(TP)}} = \frac{n_s(\Delta m)^2 \omega^5 c_R^4}{16\pi \rho^2 c_i^3 \epsilon} \int_0^{\pi/2} d\theta_s \frac{\sin\theta_s \cos^2\theta_s}{|4\epsilon(\theta_s) \cos\theta_s \sin^2\theta_s |\lambda^2 - \sin^2\theta_s|^{1/2} + \cos^2 2\theta_s|^2} \times \left(\frac{\cos^2 2\theta_s}{|D_1(0; \omega)|^2} + \frac{8\rho_i^2 \sin^2\theta_s |\lambda^2 - \sin^2\theta_s|}{\sigma^2 |D_3(0; \omega)|^2} \right). \quad (4.31)$$

The contributions of s -polarized transverse bulk waves and of Rayleigh waves to the inverse attenuation length can be evaluated in closed form using Eqs. (4.21), (4.25), and (4.26)–(4.29). The results are, respectively,

$$\frac{1}{\bar{l}^{(TS)}} = \frac{n_s(\Delta m)^2 \omega^5 c_R^4}{16\pi \rho^2 c_i^3 \epsilon |D_1(0; \omega)|^2}, \quad (4.32)$$

$$\frac{1}{\bar{l}^{(R)}} = \frac{n_s(\Delta m)^2 \omega^5 c_R^3}{32\rho^2 R^2 \rho_i^2 \sigma^2 c_i^3} \times \left(\frac{1}{|D_1(0; \omega)|^2} + \frac{\rho_i^2}{\rho_i^2} \frac{2}{|D_3(0; \omega)|^2} \right). \quad (4.33)$$

We now turn our attention to the case where the mass defects are distributed uniformly throughout the crystal. It is now necessary to multiply the energy stored per unit time in the scattered wave by the concentration of defects n_b and to integrate over x_{03} . The contribution to the inverse attenuation length from longitudinal bulk waves is then given by

$$\frac{1}{\bar{l}^{(L)}} = \frac{L_2 n_b}{dE_0/dt} \int_0^\infty dx_{03} \frac{dE_L(x_{03})}{dt}. \quad (4.34)$$

The integral over x_{03} can be evaluated analytically if we ignore the resonance situation and set $D_1(\vec{x}_0; \omega) = D_3(\vec{x}_0; \omega) = 1$. However, the results are long and cumbersome, and one is still left with the integral over θ_s to be done numerically. We content ourselves with presenting expressions which give the order of magnitude of the various contributions:

$$\frac{1}{\bar{l}^{(L)}} \approx \frac{n_b(\Delta m)^2 \omega^4 c_R}{2\pi \rho^2 c_i^3 \epsilon}, \quad (4.35)$$

$$\frac{1}{\bar{l}^{(TP)}} \approx \frac{1}{\bar{l}^{(TS)}} \approx \frac{n_b(\Delta m)^2 \omega^4 c_R}{4\pi \rho^2 c_i^3 \epsilon}, \quad (4.36)$$

$$\frac{1}{\bar{l}^{(R)}} = \frac{n_b(\Delta m)^2 \omega^4}{2\rho^2 R^2 c^4 \sigma^4}. \quad (4.37)$$

The difference in the frequency dependence of Eqs. (4.35)–(4.37) and Eqs. (4.31)–(4.33) is easily understood in a qualitative way. When the mass defects are uniformly distributed, only those defects located within the penetration depth of the

Rayleigh waves are effective in scattering. The effective defects can be characterized by a surface concentration $n_s = n_b L_R$, where the penetration depth L_R is approximately equal to c_R/ω . Substitution of this expression for n_s into Eqs. (4.31)–(4.33) yields the frequency dependence of Eqs. (4.35)–(4.37).

V. DISCUSSION

When the mass defects are localized at the surface, our results for the various contributions to the inverse attenuation length of Rayleigh waves are proportional to the square of the change in mass introduced by the defect and to the fifth power of the frequency. In this respect our results are in agreement with those of Steg and Klemens⁴ and of Sakuma.^{5,6} Like Sakuma, we have also obtained resonance behavior (see Appendix). However, our resonance behavior is somewhat different from that found by Sakuma. He found resonances when the mass defect corresponds to an impurity atom lighter than the atom of the host lattice it replaces. We find the opposite situation—i.e., resonances when the impurity atom is heavier than the host lattice atom. We believe our result is more reasonable physically than that of Sakuma. A light impurity, under proper conditions, will lead to a localized impurity mode whose frequency lies above the allowed band of frequencies for the bulk crystal. The impurity mode frequency therefore lies outside the range of Rayleigh wave frequencies. It is difficult to visualize how there can be a strong resonant interaction between a Rayleigh wave and an impurity mode whose frequency cannot equal that of the Rayleigh wave. A heavy impurity, on the other hand, can lead to a resonance mode whose frequency lies within the allowed band for the bulk crystal. In general, there will be no problem in finding a Rayleigh wave whose frequency is equal to that of the resonance mode. We interpret the peaks in the quantities $|D_1(0; \omega)|^{-2}$ and $|D_3(0; \omega)|^{-2}$ to be at the resonance mode frequencies of the heavy mass defect.

The peaks do not occur at the same frequency because the impurity mode in which the motion of the defect is perpendicular to the surface lies at a lower frequency than does the mode in which the motion of the defect is parallel to the surface.

It is of interest to evaluate the order of magnitude of the inverse attenuation length. If we consider silicon with $\rho = 2.5 \text{ g/cm}^3$, $c_R = 4.9 \times 10^5 \text{ cm/sec}$, $c_t = 5.3 \times 10^5 \text{ cm/sec}$, and $c_l = 9.5 \times 10^5 \text{ cm/sec}$, and assume that the defects are localized at the surface with $n_s = 10^{12} \text{ cm}^{-2}$ and $\Delta m = 10^{-23} \text{ g}$, we obtain for $\omega = 10^{10} \text{ Hz}$ the values $l^{(l)} = 3.1 \times 10^{15} \text{ cm}$, $l^{(tp)} = 2.1 \times 10^{15} \text{ cm}$, $l^{(ts)} = 2.1 \times 10^{15} \text{ cm}$, and $l^{(R)} = 0.77 \times 10^{15} \text{ cm}$. In these calculations, the integrals in Eqs. (4.30) and (4.31) have been taken equal to unity. We see that for the defect concentration and frequency considered, the attenuation length is extremely long. If we increase the frequency by a factor of 1000 to 10^{13} Hz , we then find $l^{(l)} = 3.1 \text{ cm}$, $l^{(tp)} = 2.1 \text{ cm}$, $l^{(ts)} = 2.1 \text{ cm}$, and $l^{(R)} = 0.77 \text{ cm}$. These lengths are moderately short, but the frequency is much higher than those used in surface-wave devices.

In the above calculations, the resonances have been neglected. Including the resonances could decrease the attenuation lengths by an order of magnitude or more at the resonance frequencies. One can, of course, also decrease the attenuation length by increasing the mass change Δm or the concentration n_s of defects. In typical situations, however, it seems likely that scattering by surface roughness⁹ will be more significant in determining the attenuation length than will scattering by mass defects.

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APPENDIX

In this Appendix we evaluate the resonance denominators $D_\alpha(\vec{x}_0; \omega)$ ($\alpha = 1, 2, 3$) which enter the expression for the scattered displacement field, Eq. (2.12), and which are defined in Eq. (2.11). We have that

$$D_\alpha(\vec{x}_0; \omega) = 1 + (\Delta m \omega^2 / \rho) G_{\alpha\alpha}(x_0, x_0; \omega). \quad (\text{A1})$$

We begin by showing that $G_{\alpha\beta}(\vec{x}, \vec{x}; \omega)$ is diagonal in α and β , and that $G_{11}(\vec{x}, \vec{x}; \omega) = G_{22}(\vec{x}, \vec{x}; \omega) \neq G_{33}(\vec{x}, \vec{x}; \omega)$. For this purpose we first note that the Green's function $G_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)$ can be written as the sum of a contribution $G_{\alpha\beta}^\infty(\vec{x}, \vec{x}'; \omega)$, which is the Green's function for an infinitely extended medium, and a contribution $\Delta G_{\alpha\beta}(\vec{x}, \vec{x}; \omega)$, which

reflects the semi-infinite nature of the elastic medium and ensures that the surface $x_3 = 0$ is stress free. The Green's function $G_{\alpha\beta}^\infty(\vec{x}, \vec{x}'; \omega)$ diverges as $\vec{x} \rightarrow \vec{x}'$, so that it must be treated separately and specially. It is to this function that we turn first.

The Green's function $G_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)$ has the Fourier expansion

$$G_{\alpha\beta}(\vec{x}, \vec{x}'; \omega) = \int \frac{d^2 k_\parallel}{(2\pi)^2} g_{\alpha\beta} \times (\vec{k}_\parallel \omega | x_3 x_3') e^{i\vec{k}_\parallel \cdot (\vec{x}_\parallel - \vec{x}'_\parallel)}, \quad (\text{A2})$$

where the Fourier coefficients in turn are expressible in terms of simpler functions $d_{\alpha\beta}(k_\parallel \omega | x_3 x_3')$, which depend on \vec{k}_\parallel only through its magnitude, through Eqs. (2.13) and (2.14). The part of $d_{\alpha\beta}(k_\parallel \omega | x_3 x_3')$ which gives rise to the Green's function $G_{\alpha\beta}^\infty(\vec{x}, \vec{x}'; \omega)$ has as its only nonzero elements⁹

$$d_{11}^\infty(k_\parallel \omega | x_3 x_3') = -\frac{k_\parallel^2}{2\alpha_t \omega^2} (e^{-\alpha_l |x_3 - x_3'|} - e^{-\alpha_t |x_3 - x_3'|}), \quad (\text{A3a})$$

$$d_{13}^\infty(k_\parallel \omega | x_3 x_3') = -\frac{ik_\parallel}{2\omega^2} \text{sgn}(x_3 - x_3') \times (e^{-\alpha_l |x_3 - x_3'|} - e^{-\alpha_t |x_3 - x_3'|}), \quad (\text{A3b})$$

$$d_{22}^\infty(k_\parallel \omega | x_3 x_3') = -\frac{e^{-\alpha_t |x_3 - x_3'|}}{2\alpha_t c_t^2}, \quad (\text{A3c})$$

$$d_{31}^\infty(k_\parallel \omega | x_3 x_3') = -\frac{ik_\parallel}{2\omega^2} \text{sgn}(x_3 - x_3') \times (e^{-\alpha_l |x_3 - x_3'|} - e^{-\alpha_t |x_3 - x_3'|}), \quad (\text{A3d})$$

$$d_{33}^\infty(k_\parallel \omega | x_3 x_3') = \frac{k_\parallel^2}{2\alpha_t \omega^2} (e^{-\alpha_l |x_3 - x_3'|} - e^{-\alpha_t |x_3 - x_3'|}). \quad (\text{A3e})$$

The functions α_l and α_t appearing in these expressions are defined by

$$\alpha_{t,l} = \begin{cases} \left(k_\parallel^2 - \frac{\omega^2}{c_{t,l}^2} \right)^{1/2}, & k_\parallel > \frac{\omega}{c_{t,l}} \\ \left(-i \frac{\omega^2}{c_{t,l}^2} - k_\parallel^2 \right)^{1/2}, & k_\parallel < \frac{\omega}{c_{t,l}} \end{cases} \quad (\text{A4a})$$

$$\left(-i \frac{\omega^2}{c_{t,l}^2} - k_\parallel^2 \right)^{1/2}, \quad k_\parallel < \frac{\omega}{c_{t,l}}. \quad (\text{A4b})$$

These definitions can be combined into the single equation

$$\alpha_{t,l} = [k_\parallel^2 - (\omega + i\eta)^2 / c_{t,l}^2]^{1/2}, \quad (\text{A5})$$

where η is a positive infinitesimal, and the branch cut in the definition of the square root is along the

negative real axis.

With the aid of the representations

$$e^{-\alpha|x_3-x'_3|} = \int \frac{dk_z}{2\pi} e^{ik_z(x_3-x'_3)} \frac{2\alpha}{\alpha^2+k_z^2}, \quad (\text{A6a})$$

$$\text{sgn}(x_3-x'_3)e^{-\alpha|x_3-x'_3|}$$

$$= - \int \frac{dk_z}{2\pi} e^{ik_z(x_3-x'_3)} \frac{2ik_z}{\alpha^2+k_z^2}, \quad (\text{A6b})$$

and Eqs. (A2), (A3), (2.15), and (2.16) we obtain for the elements of the Green's function $G_{\alpha\beta}^\infty(\vec{x}, \vec{x}'; \omega)$:

$$G_{\alpha\beta}^\infty(\vec{x}, \vec{x}'; \omega) = - \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} \left[\frac{k_\alpha k_\beta}{\omega^2} \left(\frac{1}{k^2 - \omega^2/c_t^2} - \frac{1}{k^2 - \omega^2/c_l^2} \right) + \frac{\delta_{\alpha\beta}}{c_t^2} \frac{1}{k^2 - \omega^2/c_t^2} \right]. \quad (\text{A7})$$

In the limit as $\vec{x} \rightarrow \vec{x}'$ this integral diverges at the upper limit. In order to obtain a finite result in this limit we must impose a cutoff on the integral. We do so by confining the integration to the interior of a sphere of radius k_D , the Debye sphere. Such a cutoff arises naturally in a lattice theory,

where k_D is of the order of the reciprocal of a lattice parameter, but it has to be imposed in this fashion in a continuum theory. If we utilize the spherical symmetry of the problem, we obtain

$$\begin{aligned} G_{\alpha\beta}^\infty(\vec{x}, \vec{x}'; \omega) &= - \frac{\delta_{\alpha\beta}}{6\pi^2} \int_0^{k_D} dk k^2 \left(\frac{1}{c_t^2} \frac{1}{k^2 - \omega^2/c_t^2} + \frac{2}{c_l^2} \frac{1}{k^2 - \omega^2/c_l^2} \right) \\ &= - \frac{\delta_{\alpha\beta}}{6\pi^2} \left\{ \left(\frac{1}{c_t^2} + \frac{2}{c_l^2} \right) k_D + \frac{\omega}{2} \left(\frac{1}{c_l^3} \ln \left| \frac{k_D - \omega/c_l}{k_D + \omega/c_l} \right| + \left[\frac{2}{c_t^3} \ln \left| \frac{k_D - \omega/c_t}{k_D + \omega/c_t} \right| \right] \right) \right. \\ &\quad \left. + \frac{i\pi\omega}{2} + \frac{1}{c_l^3} \left(\Theta k_D - \frac{\omega}{c_l} \right) + \frac{2}{c_t^3} \left(\Theta k_D - \frac{\omega}{c_t} \right) \right\}, \quad (\text{A8}) \end{aligned}$$

where we have used the fact that the frequency ω has an infinitesimal positive imaginary part [see Eq. (A5)].

We now turn to the contribution to $D_\alpha(\vec{x}_0; \omega)$ from $\Delta G_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)$. The latter is given by

$$\begin{aligned} \Delta G_{\alpha\beta}(\vec{x}, \vec{x}'; \omega) &= \sum_{\mu\nu} \int \frac{d^2k_\parallel}{(2\pi)^2} e^{i\vec{k}_\parallel \cdot (\vec{x}_\parallel - \vec{x}'_\parallel)} \\ &\quad \times \Delta d_{\mu\nu}(k_\parallel \omega | x_3 x'_3) \\ &\quad \times S_{\mu\nu}(k_\parallel) S_{\nu\beta}(k_\parallel), \quad (\text{A9}) \end{aligned}$$

where $\Delta d_{\mu\nu}(k_\parallel \omega | x_3 x'_3)$ is that part of $d_{\mu\nu}(k_\parallel \omega | x_3 x'_3)$ which arises from the semi-infinite nature of the elastic medium. It depends on the two-dimensional wave vector \vec{k}_\parallel only through its magnitude. We now set $\vec{x} = \vec{x}'$ and note that the only terms that survive the integration in Eq. (A9) are those whose integrands are even functions of k_1 and k_2 . In this way we obtain for the only nonzero elements of $\Delta G_{\alpha\beta}(\vec{x}, \vec{x}; \omega)$

$$\begin{aligned} \Delta G_{11}(\vec{x}, \vec{x}; \omega) &= \int \frac{d^2k_\parallel}{(2\pi)^2} \left[\hat{k}_1^2 \Delta d_{11}(k_\parallel \omega | x_3 x_3) \right. \\ &\quad \left. + \hat{k}_2^2 \Delta d_{22}(k_\parallel \omega | x_3 x_3) \right], \quad (\text{A10a}) \end{aligned}$$

$$\begin{aligned} \Delta G_{22}(\vec{x}, \vec{x}; \omega) &= \int \frac{d^2k_\parallel}{(2\pi)^2} \left[\hat{k}_1^2 \Delta d_{22}(\hat{k}_1^2 \Delta d_{22}(k_\parallel \omega | x_3 x_3)) \right. \\ &\quad \left. \times \hat{k}_2^2 \Delta d_{11}(k_\parallel \omega | x_3 x_3) \right], \quad (\text{A10b}) \end{aligned}$$

$$\Delta G_{33}(\vec{x}, \vec{x}; \omega) = \int \frac{d^2k_\parallel}{(2\pi)^2} \Delta d_{33}(k_\parallel \omega | x_3 x_3). \quad (\text{A10c})$$

On carrying out the angular integrations in these expressions we are left with the results that

$$\begin{aligned} \Delta G_{11}(\vec{x}, \vec{x}; \omega) &= \Delta G_{22}(\vec{x}, \vec{x}; \omega) \\ &= \frac{1}{4\pi} \int_0^{k_D} dk_\parallel k_\parallel \left[\Delta d_{11}(k_\parallel \omega | x_3 x_3) \right. \\ &\quad \left. + \Delta d_{22}(k_\parallel \omega | x_3 x_3) \right] \quad (\text{A11a}) \end{aligned}$$

$$\Delta G_{33}(\vec{x}, \vec{x}; \omega) = \frac{1}{2\pi} \int_0^{k_D} dk_\parallel k_\parallel \Delta d_{33}(k_\parallel \omega | x_3 x_3). \quad (\text{A11b})$$

We have again introduced a cutoff on the integrals over k_\parallel to render them convergent at the upper limit.

The expressions for $\Delta d_{\alpha\alpha}(k_\parallel \omega | x_3 x_3)$ obtained from Appendix A of Ref. 9 are

$$\begin{aligned} \Delta d_{11}(k_\parallel \omega | x_3 x_3) &= - \frac{k_\parallel^2}{2\alpha_l \omega^2} \frac{1}{r_+} (r_- e^{-2\alpha_l x_3} + \epsilon r_- e^{-2\alpha_l x_3} \\ &\quad + 2e^{-(\alpha_l + \alpha_t)x_3}), \quad (\text{A12a}) \end{aligned}$$

$$\Delta d_{22}(k_{\parallel} \omega | x_3, x_3) = -\frac{1}{2\alpha_t c_t^2} e^{-2\alpha_t x_3}, \tag{A12b}$$

$$\Delta d_{33}(k_{\parallel} \omega | x_3, x_3) = -\frac{k_{\parallel}^2}{2\alpha_t \omega^2} \frac{1}{r_+} (r_- e^{-2\alpha_t x_3} + \epsilon r_- e^{-2\alpha_t x_3} + 2e^{-(\alpha_i + \alpha_t)x_3}). \tag{A12c}$$

The functions α_i and α_t have been defined in Eqs. (A4) and (A5). The functions r_+ , r_- , and ϵ are given by

$$\epsilon = \frac{\alpha_i \alpha_t}{k_{\parallel}^2}, \quad r_{\pm}(k_{\parallel} \omega) = \frac{4\alpha_t \alpha_i k_{\parallel}^2 \pm (\alpha_t^2 + k_{\parallel}^2)^2}{4\alpha_t \alpha_i (\alpha_t^2 + k_{\parallel}^2)}. \tag{A13}$$

On substituting Eqs. (A12) and (A13) into Eqs. (A11) we obtain the results that

$$\begin{aligned} \Delta G_{11}(\vec{x}, \vec{x}; \omega) &= \Delta G_{22}(\vec{x}, \vec{x}; \omega) \\ &= \frac{k_D^3}{16\pi\omega_t^2 \zeta^2} \int_0^1 du \left\{ \frac{u}{(u - \lambda^2 \zeta^2)^{1/2}} \left[\frac{(2u - \zeta^2)^2 + 4u(u - \zeta^2)^{1/2}(u - \lambda^2 \zeta^2)^{1/2}}{(2u - \zeta^2) - 4u(u - \zeta^2)^{1/2}(u - \lambda^2 \zeta^2)^{1/2}} \right. \right. \\ &\quad \times \left(\exp[-2(u - \lambda^2 \zeta^2)^{1/2} k_D x_3] \right. \\ &\quad \left. \left. + \frac{(u - \zeta^2)^{1/2} (u - \lambda^2 \zeta^2)^{1/2}}{u} \exp[-2(u - \zeta^2)^{1/2} k_D x_3] \right) \right. \\ &\quad \left. - \frac{8(u - \zeta^2)^{1/2} (u - \lambda^2 \zeta^2)^{1/2} (2u - \zeta^2)}{(2u - \zeta^2)^2 - 4u(u - \zeta^2)^{1/2} (u - \lambda^2 \zeta^2)^{1/2}} \right. \\ &\quad \left. \times \exp \left\{ -[(u - \lambda^2 \zeta^2)^{1/2} + (u - \zeta^2)^{1/2}] k_D x_3 \right\} \right. \\ &\quad \left. - \frac{\zeta^2}{(u - \zeta^2)^{1/2}} \exp[-2(u - \zeta^2)^{1/2} k_D x_3] \right\}, \tag{A14} \end{aligned}$$

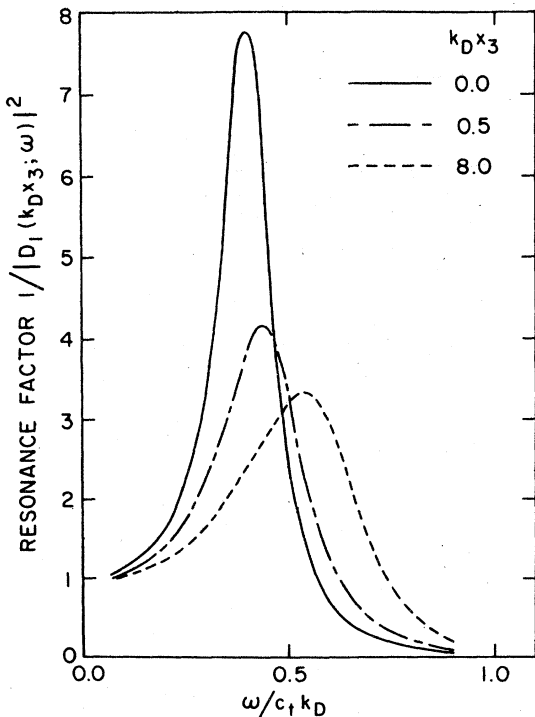


FIG. 2. Resonance factor as a function of frequency for impurity motion parallel to the surface.

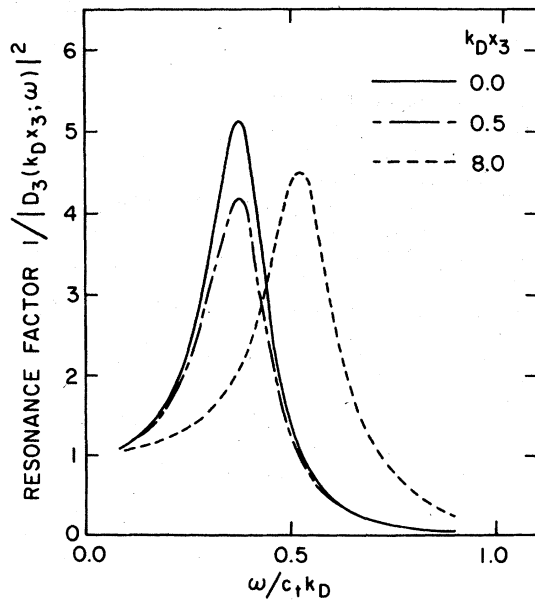


FIG. 3. Resonance factor as a function of frequency for impurity motion perpendicular to the surface.

$$\begin{aligned}
\Delta G_{33}(\vec{x}, \vec{x}; \omega) &= \frac{k_D^3}{8\pi\omega_t^2 \xi^2} \int_0^1 du \frac{u}{(u - \xi^2)^{1/2}} \left[\frac{(2u - \xi^2)^2 + 4u(u - \xi^2)^{1/2}(u - \lambda^2 \xi^2)^{1/2}}{(2u - \xi^2)^2 - 4u(u - \xi^2)^{1/2}(u - \lambda^2 \xi^2)^{1/2}} \right. \\
&\quad \times \left(\exp[-2(u - \xi^2)^{1/2} k_D x_3] + \frac{(u - \xi^2)^{1/2}(u - \lambda^2 \xi^2)^{1/2}}{u} \exp[-2(u - \lambda^2 \xi^2)^{1/2} k_D x_3] \right) \\
&\quad \left. - \frac{8(u - \xi^2)^{1/2}(u - \lambda^2 \xi^2)^{1/2}(2u - \xi^2)}{(2u - \xi^2)^2 - 4u(u - \xi^2)^{1/2}(u - \lambda^2 \xi^2)^{1/2}} \exp\{-[(u - \lambda^2 \xi^2)^{1/2} + (u - \xi^2)^{1/2}]k_D x_3\} \right].
\end{aligned} \tag{A15}$$

In obtaining these expressions we have introduced the notation

$$\xi = \frac{\omega + i\eta}{c_t k_D}, \quad \omega_t = c_t k_D, \quad \lambda = c_t / c_l. \tag{A16}$$

Although the integrals in Eqs. (A14) and (A15) can be evaluated analytically when $x_3 = 0$, the results are cumbersome. We have therefore evaluated these integrals numerically, as functions of ω/ω_t , for several values of λ and $k_D x_3$. Simpson's rule was used, with 100 divisions of the integration interval (0, 1). A value of $10^{-3}\omega_t$ was chosen for the quantity η , and the integrations were carried out in complex arithmetic. The square roots $(u - \xi^2)^{1/2}$ and $(u - \lambda^2 \xi^2)^{1/2}$ were always evaluated in such a way that their real parts were positive, which assured the satisfaction of Eq.

(A4). The results of these calculations were combined with that given by Eq. (A8), and substituted into Eq. (A1) to yield $D_\alpha(\vec{x}_0; \omega)$. Results for $|D_1(\vec{x}_0; \omega)|^{-2}$ and $|D_3(\vec{x}_0; \omega)|^{-2}$ as functions of ω are presented in Figs. 2 and 3 for several different values of $k_D x_3$ with $\lambda = 1/\sqrt{3}$ and $\Delta m_D^3/\rho = 50$. In each of these figures, we see that there is a resonance peak whose frequency at the maximum increases as the impurity is moved from the surface into the bulk. At the surface, the peak frequency is somewhat smaller for the impurity motion perpendicular to the surface than parallel to the surface. This indicates that the effective force constant governing the impurity motion perpendicular to the surface is less than that governing the motion parallel to the surface. A similar effect is found¹⁰ in the mean-square displacements of surface atoms.

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