Surfon–Mass-Defect Scattering

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(Received 24 July 1972)

The scattering of surfons by point mass defects in a solid surface is calculated in terms of field-theoretical scattering theory. Scattering cross sections for incident Rayleigh-mode surfons into other Rayleigh-mode surfons and into one with a total-reflection mode are estimated as functions of incident frequency. It is shown that both of these cross sections have typical resonance structure in the frequency region $\omega \simeq (1-3) \times 10^{13}$ sec^{-1}.

Quantization of elastic surface waves has recently been done by Ezawa,[1] who constructed a complete orthogonal set of the eigenmodes of elastic waves in a half-space with a stress-free plane boundary. The real surface of solids, however, is rather rough, so that surfons, the quanta of elastic surface waves, will be scattered by the surface irregularities considerably. Scattering of Rayleigh waves by surface mass defects has already been discussed by Steg and Klemens[2] in a perturbative approximation, showing that the scattering varies as the fifth power of the frequency.

It is well known that there exists resonant scattering of lattice waves by point defects in crystals. Even in the presence of the surface boundary, we anticipate the resonance scattering of surface elastic waves by point defects localized in the solid surface; and we should, therefore, take into account the higher-order effects in calculating the scattering amplitudes. However, the presence of a boundary surface makes it somewhat difficult to obtain a scattering amplitude by means of the lattice Green's-function method.[3]

For this purpose, the present author and Nakayama proposed previously an alternative approach[4] for calculating the scattering amplitude, which was originally developed by Chew and Low[5] for meson scattering by a static source.

In this Letter, we apply this formalism to investigate surfon–mass-defect scattering and calculate the scattering cross section in the isotropic-elastic-continuum approximation. We assume the solid occupies the half-space $z \geqslant 0$ with a stress-free surface $z=0$. For simplicity, we deal with a point mass defect lying in the surface.

We can expand the displacement $\vec{u}(\vec{r},t)$ at a point $\vec{r}=(\vec{\rho},z)$ and a time t in terms of eigenmodes,[1]

$$\vec{u}(\vec{r},t)=\sum_J (8\pi^2\rho\omega_J)^{-1/2} \times[a_J\vec{u}^{(J)}(z)\exp^{(i\vec{k}\cdot\vec{\rho}-i\omega_J t)}+\text{H.c.}], \tag{1}$$

where ρ is the density of the crystal, J is the set of quantum numbers, and a_J is the annihilation operator of mode J. J is composed of three quantum numbers: the wave vector $\vec{k}$ in the x-y plane, the propagation velocity c in the x-y plane, and a symbol m to label the five eigenmodes of surface elastic waves in a half-space; that is, $J=\{\vec{k},c,m\}$.

Since the point mass defect is assumed to be localized in the solid surface, it would be enough to take into account only two modes: the Rayleigh mode and the mode with total reflection, among five modes which form a complete orthogonal set of the eigenmodes. The other three modes, having only oscillating wave functions at a distance z from the surface, will contribute less to scattering in the high-frequency region.

Concrete expressions of the wave function $\vec{u}^{(J)}(z)$ for the Rayleigh mode ($m=R$) and the mode with total reflection ($m=T$) are explicitly given in Ref. 1. Therefore the relevant interaction Hamiltonian of surfons with point mass defect can be obtained by inserting $\vec{u}=\vec{u}_R+\vec{u}_T$ into $H'=\frac{1}{2}\Delta M(d\vec{u}/dt)^2$, where $\vec{u}_R$ and $\vec{u}_T$ are displacements due to individual Rayleigh-mode and total-reflection-mode surfons. ΔM is the difference between the mass of defect and the average mass of the atoms. Thus we have to consider the two kinds of scattering processes for incident Rayleigh-mode surfons:

$$R+\Delta M \to R+\Delta M, \tag{2a}$$

$$R+\Delta M \to T+\Delta M. \tag{2b}$$

The scattering amplitudes for the processes (2a) and (2b) are defined as

$$T_J(J')\equiv\langle\psi_{J'}{}^{-}|V_J|\psi_0\rangle, \qquad R_J(J')\equiv\langle\psi_{J'}{}^{-}|V_J{}^{\dagger}|\psi_0\rangle, \tag{3}$$

where

$$V_J=[H',a_J], \quad J=\{\vec{k},c_R,R\},$$

$$J'=\{\vec{k}',c_R,R\} \text{ or } \{\vec{k}',c',T\}.$$

The state vector $|\psi_J^-\rangle$ is defined as an eigenstate of the total Hamiltonian composed of a single mass defect plus one J-mode surfon with an outgoing wave. $|\psi_0\rangle$ represents just the ground eigenstate of a single mass defect. Thus the relevant scattering amplitude for $J \to J'$ is $T_J(J')$. c_R is given as the solution of

$$4\{[1-(c_R/c_t)^2][1-(c_R/c_l)^2]\}^{1/2} = [2-(c_R/c_t)^2]^2,$$

where c_t and c_l are the transverse and longitudinal sound velocities in bulk crystals.

Following the standard method developed in Ref. 4, we obtain integral equations for the amplitudes (3), using a one-surfon approximation in the intermediate state:

$$\begin{aligned} T_J(J') &= T_J{}^{\mathrm{B}}(J') - \sum_{J''}\left[\frac{R_J{}^*(J'')R_{J'}(J'')}{\omega_{J''}+\omega_{J'}} + \frac{T_{J'}{}^*(J'')T_J(J'')}{\omega_{J''}-\omega_{J'}-i\epsilon}\right], \\ R_J(J') &= R_J{}^{\mathrm{B}}(J') - \sum_{J''}\left[\frac{T_J{}^*(J'')R_{J'}(J'')}{\omega_{J''}+\omega_{J'}} + \frac{T_{J'}{}^*(J'')R_J(J'')}{\omega_{J''}-\omega_{J'}-i\epsilon}\right], \end{aligned} \tag{4}$$

$T_J{}^{\mathrm{B}}(J')$ and $R_J{}^{\mathrm{B}}(J')$ being the amplitudes in the Born approximation. In Eqs. (4), we may safely neglect the first term in the bracket on the right-hand side, since the energy denominator of that term does not have a zero. Therefore, we need only solve the following integral equations for $T_J(J')$:

$$T_J(J') = T_J{}^{\mathrm{B}}(J') - \sum_{J''}\frac{T_{J'}{}^*(J'')T_J(J'')}{\omega_{J''}-\omega_{J'}-i\epsilon}. \tag{5}$$

We try to obtain an approximate solution of Eq. (5) by replacing one of the scattering amplitudes in the integral with the amplitude in the Born approximation. This approximation is shown diagrammatically in Fig. 1, and is given analytically by

$$T_J(J') = T_J{}^{\mathrm{B}}(J') - \sum_{J''}\frac{T_{J'}{}^{\mathrm{B}*}(J'')T_J(J'')}{\omega_{J''}-\omega_{J'}-i\epsilon}. \tag{6}$$

Then, the solutions of Eq. (6) can easily be obtained by the standard method, and we have the following expressions for the cross sections:

$$\sigma_{R\to R}(\omega) = \frac{(\Delta M)^2 D_1{}^2\omega^5}{4\pi^2\rho^2 c_R{}^5}\left[\frac{2|1-3N|^2}{|(1+L)(1+N)-4LN|^2} + \frac{(D_2/D_1)^2|1-3N'|^2}{|(1+L')(1+N')-4L'N'|^2}\right], \tag{7}$$

$$\sigma_{R\to T}(\omega) = \frac{(\Delta M)^2 C_1 D_1\omega^5}{\pi^2\rho^2 c_R{}^5}\left[\frac{2}{|(1+L)(1+N)-4LN|^2} + \frac{C_2D_2/C_1D_1}{|(1+L')(1+N')-4L'N'|^2}\right], \tag{8}$$

where

$$L = \frac{\Delta M\, D_1}{2\pi\rho}\left(\frac{\omega_{\max}}{c_R}\right)^3 f(x), \quad L' = \frac{\Delta M\, D_2}{2\pi\rho}\left(\frac{\omega_{\max}}{c_R}\right)^3 f(x),$$

$$N = \frac{\Delta M\, C_1}{2\pi\rho}\left(\frac{\omega_{\max}}{c_R}\right)^3 f(x), \quad N' = \frac{\Delta M\, C_2}{2\pi\rho}\left(\frac{\omega_{\max}}{c_R}\right)^3 f(x),$$

$$f(x) = \tfrac{1}{2} + \tfrac{1}{3}x + x^2 + x^3\ln[(1-x)/x] + i\pi x^3,$$

$$x = \omega/\omega_{\max}.$$

C_1, C_2, D_1, and D_2 are some dimensionless constants which depend upon c_l, c_t, and c_R. $\omega_{\max}$ is the maximum surfon frequency, corresponding to the Debye frequency in the bulk phonon case.

Resonant parts in the square bracket on the right-hand side of Eqs. (7) and (8) represent the higher-order rescattering effect of surfons with static mass defects, and thus it is seen that scattering in lowest-order perturbation theory varies as the fifth power of the frequency, as predicted in Ref. 2.

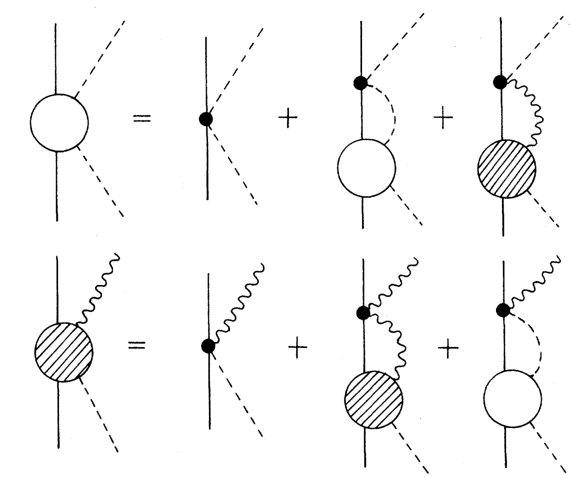

FIG. 1. Graphical schemes for the simultaneous integral equations (6). Solid line, physical mass defect; dashed line, Rayleigh-mode surfon; wavy line, that with a total-reflection mode. Open and shaded circles, physical amplitudes for the processes (2a) and (2b), respectively. Closed circle, amplitude in Born approximation.

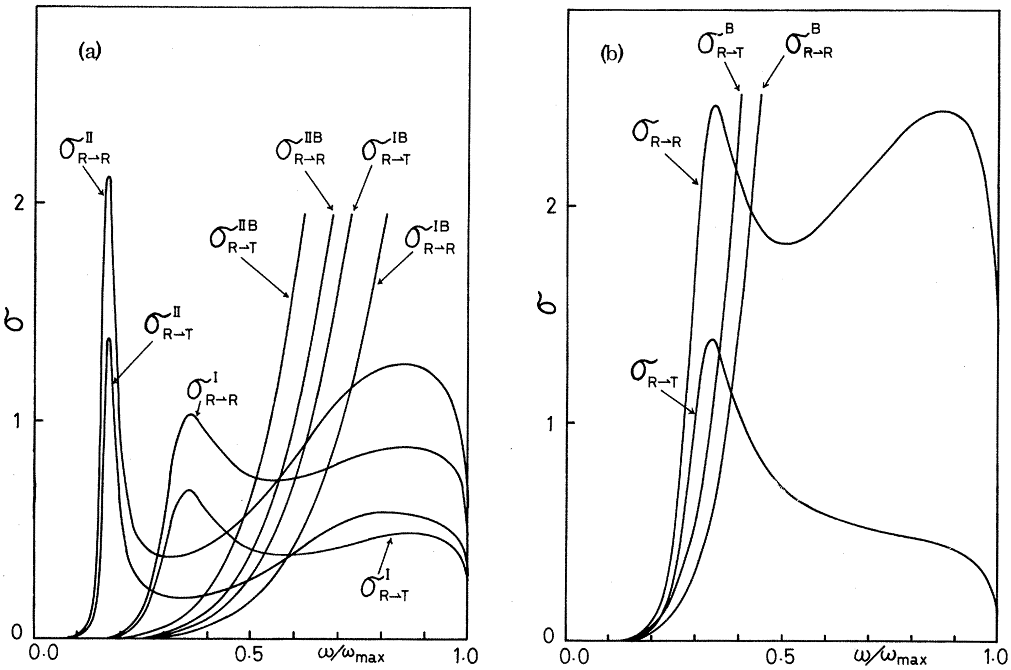

FIG. 2. (a) Surfon–mass-defect scattering cross section as a function of frequency in units of ω_{max} for $\Delta M = -4m$ and $-6m$, where m is the neutron mass. Case I, $\Delta M = -4m$; case II, $\Delta M = -6m$. The superscript B refers to the Born approximation. (b) Same as in (a) but for $\Delta M = -20m$.

In order to show an actual frequency dependence of the cross sections (7) and (8), we take the following typical values of parameters for Si: $\rho = 2.5$ g/cm^3, $c_t = 5.3\times10^5$ cm/sec, $c_l = 9.5\times10^5$ cm/sec, and $c_R = 4.9\times10^5$ cm/sec. Here, we assume the maximum frequency ω_{max} to be 0.75×10^{14} sec^{-1}, which may be somewhat smaller than the Debye frequency.

The cross sections in the present approximation are shown in Figs. 2(a) and 2(b) for various masses of static defects together with the cross section in the Born approximation.

As there are two different kinds of resonance terms in Eqs. (7) and (8), we have two typical resonance scatterings for the mass ranges $4m \leq -\Delta M \leq 7m$ and $16m \leq -\Delta M \leq 34m$, respectively, in the frequency range $\omega = 0.15\omega_{max}$–$0.4\omega_{max}$ (m is the neutron mass). These characteristic features agree qualitatively with the results obtained in Ref. 4, in which only the scattering of Rayleigh-mode surfons was considered.

Defining a partition ratio δ as in Ref. 2, which is the rate of scattering into other Rayleigh modes relative to scattering into the total-reflection modes, $\delta = \sigma_{R\to T}/\sigma_{R\to R}$, we have a frequency-independent ratio in the Born approximation which gives a value around 1.6. If, on the other hand, we take higher-order rescattering effects into account, the partition ratio decreases and gives a value smaller than 1 as is seen in Figs. 2(a) and 2(b). Therefore, we conclude that the rescattering effects enhance the scattering into other Rayleigh-mode surfons. It should also be emphasized that resonance scattering appears for a static surface defect of lighter mass than that of the host atoms in surfon–mass-defect scattering.

The author thanks T. Nakayama for discussions. The numerical calculations were performed using a FACOM 230-60 computer at the Computer Center of Hokkaido University.

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