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Surface-wave scattering by isotopic impurities in solids*

D. K. Dacol† and A. H. Zimerman
Instituto de Física Teórica, São Paulo, Brazil
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Exact expressions for the transition amplitudes for the scattering of surface waves by point-mass defects are obtained by methods which are similar to those used in connection with the Wentzel model of field theory.

Interest in elastic surface waves has been growing in recent years, mainly in connection with studies of the transport properties of electrons in semiconductor inversion layers.[1] Lately, the scattering of such waves by mass defects has also been subject of interest. For instance, Steg and Klemens[2] studied the scattering of Rayleigh waves by perturbation theory and its attenuation as function of the depth of the impurity.

After Ezawa's[3] quantization of the elastic waves in a solid having a stress-free plane boundary and occupying a half-space, Sakuma[4] studied the scattering of surface waves by a mass defect in this medium by considering the mass defect as a scattering center for the surfons (the quanta of the waves in this medium). Using a version of the Chew-Low equation adapted to the surfon-isotopic impurity-scattering problem, he obtained an approximate expression for the transition amplitude when the isotopic impurity is localized on the solid's surface.

In this paper we present an exact solution to this problem obtained through a canonical transformation method which was successfully used in the study of the Wentzel model and in the phonon–isotopic-impurity scattering problem.[5,6]

Let us take a crystal lattice compounded of equal atoms (one in each cell) occupying a half-space ($z>0$) and having a stress-free boundary (the plane $z=0$) and then consider the case in which one of the atoms is replaced by an isotope. The Hamiltonian for the lattice with isotopic impurity is[5]

$$H=H_0-[\Delta M/(M+\Delta M)]\,\vec{p}^2(r_0)/2M\ . \qquad (1)$$

In Eq. (1), M is the mass of the atoms in the crystal lattice, $M+\Delta M$ is the mass of the isotope (which is supposed to be localized at the lattice site $\vec{r}_0$), $\vec{p}(\vec{r})$ is the momentum of the atom at the lattice site $\vec{r}$ [$\vec{u}(\vec{r})$ is the displacement vector of this atom], and H_0 is the Hamiltonian for the perfect lattice.

The Hamiltonian (1) will be studied in the acoustical approximation; that is, we will treat the crystal lattice as if it were an isotropic elastic continuum but with the restriction that the elastic wave frequencies are in the interval $0<\omega<\omega_{\max}$. Ezawa's surfon field expansion for $\vec{u}(\vec{r})$ and $\vec{p}(\vec{r})$ will be used:

$$\vec{u}(\vec{r})=\sum_J\left(\frac{1}{2\rho\omega_J}\right)^{1/2}[a_J\vec{u}^{(J)}(\vec{r})+a_J^\dagger u^{(J)*}(\vec{r})]\,,$$
$$\vec{p}(\vec{r})=-iM\sum_J\left(\frac{\omega_J}{2\rho}\right)^{1/2}[a_J\vec{u}^{(J)}(\vec{r})-a_J^\dagger\vec{u}^{(J)*}(\vec{r})]\,. \qquad (2)$$

In Eqs. (2), $J=(\vec{k},c,m)$ is a suitable set of quantum numbers for the surfons, $\vec{k}=(k_1,k_2,0)$ is a wave vector parallel to the plane $z=0$, c is a phase velocity ($\omega_J=kc$), and m specifies the propagation mode. The functions $\vec{u}^J(\vec{r})$ are given by

$$\vec{u}^{(J)}(\vec{r})=\vec{u}_J(z)\,e^{i\vec{k}\vec{r}}/S^{1/2}\ , \qquad (3)$$

where S is an area on the plane $z=0$ and the functions $e^{i\vec{k}\vec{r}}/S^{1/2}$ satisfy periodic boundary conditions on the limits of S, the expressions for $\vec{u}_J(z)$ can be read from Ezawa's[3] work.[7] The definition of the sum over J in Eq. (1) is

$$\sum_J f(J)=\frac{S}{(2\pi)^2}\int d^2k\left(\sum_{mR}\int_{\Gamma_m}\frac{dc}{c}f(\vec{k},c,m)+f(\vec{k},C_R,R)\right)\ . \qquad (4)$$

Γ_m denotes the range of the phase velocities for the mode m. The operators a_J and $a_J^\dagger$ are annihilation and creation operators for the surfons; they obey the usual Bose commutation relations

$$[a_J,a_{J'}]=[a_J^\dagger,a_{J'}^\dagger]=0\,,\quad [a_J,a_{J'}^\dagger]=\delta_{JJ'}\ ,$$
$$\delta_{JJ'}=\delta_{\vec{k}\vec{k}'}\,\delta(c,c')\delta_{mm'}\ , \qquad (5)$$

with

$$\delta_{\vec{k}\vec{k}'}=\frac{1}{S}\int_S e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\,dS\ ,$$

$\delta(c,c')=c\,\delta(c-c')$ if c and c' belong to the continuous spectrum, $\delta(c,c')=\delta_{cc'}$ if c or c' belongs to the discrete spectrum, and $\delta_{cc'}$ and $\delta_{mm'}$ are the usual Kronecker deltas.

From Eqs. (1) and (2) [with $\vec{r}_0=(0,0,z)$], we get

$$H=H_0+H'\ ,$$

with

$$H_0=\sum_J \omega_J a_J^\dagger a_J\ , \tag{6}$$

$$H'=-\lambda\sum_{JJ'}(\omega_J\omega_{J'})^{1/2}(a_J\vec{u}_J(z)-a_J^\dagger\vec{u}_J^*(z))\times(a_{J'}\vec{u}_{J'}(z)-a_{J'}^\dagger\vec{u}_{J'}^*(z))\ , \tag{7}$$

$$\lambda=-[M/(M+\Delta M)](\Delta M/4\rho S)\ .$$

In order to exhibit the solution of this problem we will follow closely the treatment given by Chevalier and Rideau[8] to the Wentzel's model. According to them we introduce the operators

$$A_J=\sum_{J'}\{\Gamma_1(JJ')a_{J'}+\Gamma_2(JJ')a_{J'}^\dagger\}\ ,$$
$$A_J^\dagger=\sum_{J'}\{\Gamma_1^*(JJ')a_{J'}^\dagger+\Gamma_2^*(JJ')a_{J'}\}\ . \tag{8}$$

The asterisk indicates complex conjugation. The coefficients $\Gamma_1(JJ')$ and $\Gamma_2(JJ')$ are determined by imposing the constraint

$$[H,A_J]=-\omega_J A_J\ . \tag{9}$$

From Eqs. (8) and (9), it follows that

$$(\omega_J-\omega_{J'})\Gamma_1(JJ')=2\lambda\vec{u}_{J'}(z)\cdot\left(\sum_{J_1}(\omega_{J_1}\omega_{J'})^{1/2}[\Gamma_1(JJ_1)\vec{u}_{J_1}^*(z)+\Gamma_2(JJ_1)\vec{u}_{J_1}(z)]\right),$$
$$(\omega_J+\omega_{J'})\Gamma_2(JJ')=-2\lambda\vec{u}_{J'}(z)\cdot\left(\sum_{J_1}(\omega_{J_1}\omega_{J'})^{1/2}[\Gamma_1(JJ_1)\vec{u}_{J_1}^*(z)+\Gamma_2(JJ_1)\vec{u}_{J_1}(z)]\right). \tag{10}$$

The solution of Eqs. (10) (with the proper boundary conditions) are

$$\Gamma_1(JJ')=\delta_{JJ'}+\frac{2(\omega_J\omega_{J'})^{1/2}\vec{u}_{J'}\cdot\vec{F}_J}{\omega_J-\omega_{J'}-i\epsilon}\ ,$$
$$\Gamma_2(JJ')=-\frac{2(\omega_J\omega_{J'})^{1/2}\vec{u}_{J'}^*\cdot\vec{F}_J}{\omega_J+\omega_{J'}-i\epsilon}\ , \tag{11}$$

where ϵ is a positive infinitesimal. The vector $\vec{F}_J$ satisfies the following equation:

$$\vec{F}_J=\vec{u}_J^*+2\lambda\sum_{J_1}\omega_{J_1}\left(\frac{(\vec{F}_J\cdot\vec{u}_{J_1})\vec{u}_{J_1}^*}{\omega_J-\omega_{J_1}-i\epsilon}-\frac{(\vec{F}_J\cdot\vec{u}_{J_1}^*)\vec{u}_{J_1}}{\omega_J+\omega_{J_1}-i\epsilon}\right). \tag{12}$$

The solution of Eq. (12) is obtained by noting that

$$\sum_J[\vec{A}(\omega_J)\cdot\vec{u}_J(z)][\vec{u}_J^*(z)\cdot B(\omega_J)]=\frac{1}{2}\int_0^{\omega_{\max}}[\vec{A}(\omega)\cdot\vec{B}(\omega)-(\vec{n}\cdot\vec{A}(\omega))(\vec{n}\cdot\vec{B}(\omega))]\nu(\omega)d\omega+\int_0^{\omega_{\max}}[\vec{n}\cdot\vec{A}(\omega)][\vec{n}\cdot\vec{B}(\omega)]\mu(\omega)d\omega\ . \tag{13}$$

$\vec{n}$ is a unit vector along the z axis and

$$\nu(\omega)=\sum_J(|\vec{u}_J(z)|^2-|\vec{n}\cdot\vec{u}_J(z)|^2)\delta(\omega-\omega_J)\ , \tag{14}$$

$$\mu(\omega)=\sum_J|\vec{n}\cdot\vec{u}_J(z)|^2\delta(\omega-\omega_J)\ . \tag{15}$$

From Eqs. (12) and (13) we have

$$\vec{F}_J(z)=\frac{\vec{u}_J^*(z)}{P-(\omega_J)}+\left(\frac{1}{Q_-(\omega_J)}-\frac{1}{P_-(\omega_J)}\right)[\vec{n}\cdot\vec{u}_J^*(z)]\vec{n}\ , \tag{16}$$

with

$$P_\pm(\omega)=\lim_{\epsilon\to0^+}P(\omega\pm i\epsilon)\ ,\quad Q_\pm(\omega)=\lim_{\epsilon\to0^+}Q(\omega\pm i\epsilon)\ , \tag{17}$$

where

$$P(\omega)=1+2\lambda\int_0^{\omega_{\max}}\frac{x^2\nu(x)\,dx}{x^2-\omega^2}\ , \tag{18}$$

$$Q(\omega)=1+4\lambda\int_0^{\omega_{\max}}\frac{x^2\mu(x)\,dx}{x^2-\omega^2}\ . \tag{19}$$

$P(\omega)$ and $Q(\omega)$ are analytic functions of the complex variable ω, with a cut along the real interval $-\omega_{\max}<\omega<\omega_{\max}$. When these functions have zeros, they are located either on the imaginary axis or on the real axis. In this paper we will assume that the functions $P(\omega)$ and $Q(\omega)$ have no zeros; that is, we will assume satisfied (simultaneously) the conditions

$$\left(\frac{M}{2\rho S}\int_0^{\omega_{\max}}\nu(\omega)d\omega-1\right)^{-1}>\frac{\Delta M}{M}>0\ ,$$
$$\left(\frac{M}{\rho S}\int_0^{\omega_{\max}}\mu(\omega)d\omega-1\right)^{-1}>\frac{\Delta M}{M}>0\ . \tag{20}$$

It can be shown that in this case we have

$$H=\sum_J\omega_J A_J^\dagger A_J\ , \tag{21}$$

with

$$[A_J,A_{J'}]=[A_J^\dagger,A_{J'}^\dagger]=0\ ,\quad [A_J,A_{J'}^\dagger]=\delta_{JJ'}\ . \tag{22}$$

As we want the transition amplitude for the scattering of surfons by the isotopic impurity, our next step will be the determination of the asymptotic annihilation and creation operators. For the incoming and outgoing operators, we have

$$a_{\substack{\text{in}\\\text{out}}}(J)=\lim_{t\to\infty} a_J(t)\,e^{it\omega_J}\,, \tag{23}$$

where $a_J(t)$ is the a_J operator in the Heisenberg picture. It is easy to show that

$$a_J(t)=\sum_{J'}\{\Gamma_1^*(J'J)A_{J'}e^{-it\omega_{J'}}-\Gamma_2(J'J)A_{J'}^{\dagger}e^{it\omega_{J'}}\}. \tag{24}$$

Using Eqs. (23) and (24), we get

$$a_{\substack{\text{in}\\\text{out}}}(J)=A_J-\lim_{t\to\mp\infty}\left(\sum_{J'}A_{J'}G_1(J'J)i\int_{-\infty}^{t}dv\,e^{iv(\omega_J-\omega_{J'})}-\sum_{J'}A_{J'}^{\dagger}G_2(J'J)i\int_{-\infty}^{t}dv\,e^{iv(\omega_J+\omega_{J'})}\right),$$

with

$$G_1(J'J)=(\omega_J-\omega_{J'})\Gamma_1^*(J'J)\,,$$
$$G_2(J'J)=-(\omega_J+\omega_{J'})\Gamma_2(J'J)\,. \tag{25}$$

Doing the limits, we obtain

$$a_{\text{in}}(J)=A_J\,, \tag{26}$$

$$a_{\text{out}}(J)=\sum_{J'}(\delta_{JJ'}-2\pi i\,\delta(\omega_j-\omega_{J'})T_{JJ'})A_{J'}\,, \tag{27}$$

with

$$T_{JJ'}=2\lambda(\omega_J\omega_{J'})^{1/2}\left[\frac{\vec{u}_J^*(z)\cdot\vec{u}_{J'}(z)}{P+(\omega_J)}+\left(\frac{1}{Q+(\omega_J)}-\frac{1}{P+(\omega_J)}\right)[\vec{n}\cdot\vec{u}_J^*(z)][\vec{n}\cdot\vec{u}_{J'}(z)]\right]. \tag{28}$$

The S-matrix element for scattering of a surfon by the isotopic impurity is

$$S_{JJ'}=\langle 0|a_{\text{out}}(J)a_{\text{in}}^{\dagger}(J')|0\rangle\,,$$

where $|0\rangle$ is the physical vacuum $(A_J|0\rangle=0)$. From Eqs. (26) and (27) it follows

$$S_{JJ'}=\delta_{JJ'}-2\pi i\,\delta(\omega_J-\omega_{J'})T_{JJ'}\,, \tag{29}$$

with $T_{JJ'}$ given by Eq. (28). Equations (26) and (27) tell us that the commutator $[a_{\text{out}}(J),a_{\text{in}}^{\dagger}(J')]$ is a c number which implies that the S-matrix elements between states differing by the number of surfons are equal to zero and so, the total number of surfons is conserved in surfon–isotopic-impurity scattering. From Eqs. (28) we can, for instance, obtain the probability for the transition of a Rayleigh mode to other modes or the total cross section for the scattering of one surfon on the impurity which is given by

$$\sigma(\omega_J)=\pi\left(\frac{\Delta M}{2\rho[1+\Delta M/M]}\right)^2\left[\frac{|\vec{u}_J(z)|^2}{|P+(\omega_J)|^2}P(\omega_J)+\left(\frac{q(\omega_J)}{|Q+(\omega_J)|^2}-\frac{P(\omega_J)}{|P+(\omega_J)|^2}\right)|\vec{n}\cdot\vec{u}_J(z)|^2\right]\times\theta(\omega_{\max}-\omega_J)\,, \tag{30}$$

$$P(\omega_J)=\omega_J\nu(\omega_J)/S\,,\quad q(\omega_J)=\omega_J\mu(\omega_J)/S\,.$$

In Ref. 4, the author obtained the following system of equations for the amplitude $T_{JJ'}$:

$$T_{JJ'}=\langle 0|[a_J,V_{J'}]|0\rangle-\sum_n\left(\frac{T_{nJ}^*T_{nJ'}}{E_n-\omega_J-i\epsilon}+\frac{R_{nJ'}R_{nJ}}{E_n+\omega_J+i\epsilon}\right), \tag{31}$$

$$R_{JJ'}=\langle 0|[a_J,V_{J'}^{\dagger}]|0\rangle-\sum_n\left(\frac{T_{nJ}^*R_{nJ'}}{E_n-\omega_J-i\epsilon}+\frac{T_{nJ'}^*R_{NJ}}{E_n+\omega_J+i\epsilon}\right), \tag{32}$$

with

$$T_{nJ}=\langle\psi_n-|V_J|0\rangle\,,\quad R_{nJ}=\langle\psi_n-|V_J^{\dagger}|0\rangle\,, \tag{33}$$

$$V_J=-2\lambda\cdot\vec{u}_J(z)\sum_{J'}(\omega_J\omega_{J'})^{1/2}(a_{J'}\vec{u}_{J'}(z)-a_{J'}^{\dagger}\vec{u}_{J'}^*(z)). \tag{34}$$

In the above equations $\sum_n$ means a sum over the complete set $\{|\psi_n-\rangle\}$ of eigenstates of H with eigenvalues $\{E_n\}$ (the index n indicates the number of surfons and their states). For the states $|\psi_n-\rangle$, we have

$$|\psi_n-\rangle=\frac{1}{n!}\,a_{\text{out}}^{\dagger}(J_1)\cdots a_{\text{out}}^{\dagger}(J_n)|0\rangle\,. \tag{35}$$

From Eqs. (33)–(35), we get

$$T_{nJ'}=\delta_{n1}T_{J_1J'}\,,\quad R_{nJ'}=\delta_{n1}R_{J_1J'}\,; \tag{36}$$

that is, $T_{nJ'}=R_{nJ'}=0$ if the number of surfons in the state $|\psi_n-\rangle$ is not equal to one. The expression for $R_{JJ'}$ is

$$R_{JJ'}=\langle 0|a_{\text{out}}(J)V_{J'}^{\dagger}|0\rangle=-2\lambda(\omega_J\omega_{J'})^{1/2}\times\left[\frac{\vec{u}_J^*(z)\cdot\vec{u}_{J'}^*(z)}{P+(\omega_J)}+\left(\frac{1}{Q+(\omega_J)}-\frac{1}{P+(\omega_J)}\right)\times[\vec{n}\cdot\vec{u}_J^*(z)][\vec{n}\cdot\vec{u}_{J'}^*(z)]\right]. \tag{37}$$

From Eqs. (31), (32), and (36), we see that $T_{JJ'}$ and $R_{JJ'}$ must satisfy the following equations:

$$T_{JJ'}=2\lambda(\omega_J\omega_{J'})^{1/2}\vec{u}_J(z)\cdot\vec{u}_{J'}^*(z)-\sum_{J'}\left(\frac{T_{J_1J}^*T_{J_1J'}}{\omega_{J_1}-\omega_J-i\epsilon}+\frac{R_{J_1J}^*T_{J_1J}}{\omega_{J_1}+\omega_J+i\epsilon}\right), \tag{38}$$

$$R_{JJ'}=-2\lambda(\omega_J\omega_{J'})^{1/2}\vec{u}_J^*(z)\cdot\vec{u}_{J'}^*(z)-\sum_{J'}\left(\frac{T_{J_1J}^*R_{J_1J'}}{\omega_{J_1}-\omega_J-i\epsilon}+\frac{T_{J_1J'}^*R_{J_1J}}{\omega_{J_1}+\omega_J+i\epsilon}\right). \tag{39}$$

It is not difficult to verify that the expressions (28) and (37) for $T_{JJ'}$ and $R_{JJ'}$ satisfy Eqs. (38) and (39).

In summary, by using a canonical transformation method, we have solved the surfon–isotopic-impurity scattering problem and obtained a solution to the coupled Chew-Low equations satisfied by the transition amplitude in this problem. We have also shown that only the one-surfon intermediate states contribute to the sums of the right-hand side of Eqs. (31) and (32) and so, to restrict the sum in Eqs. (31) and (32) to one surfon states only is not an approximation (as Sakuma[4] had thought) but an exact procedure.

If Eqs. (20) are not satisfied, then $P(\omega)$ and $Q(\omega)$ will have zeros. The real zeros will correspond to the "localized modes," while the imaginary zeros will correspond to instabilities of the system. These problems are presently being studied.

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[7]Please note that [denoting $\vec{u}_J^E(z)$ the expressions presented by Ezawa (Ref. 3)] $\vec{u}_J(z)=c^{1/2}\vec{u}_J^E(z)$ except for the mode $m=R$ (Rayleigh mode), where we have $\vec{u}_J(z)=\vec{u}_J^E(z)$. The component indexes 1, 2, and 3 in Ezawa's work must be understood as indicating components of $\vec{u}_J$ along the directions $\vec{K}/K$, $\vec{n}\times\vec{K}/k$ and $\vec{n}$, respectively, $\vec{n}$ being the unit vector along the z axis.

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