Surface waves on two-dimensional rough Neumann surfaces

W. Zierau \textsuperscript{a}, M.A. Leyva-Lucero \textsuperscript{b}, A.A. Maradudin \textsuperscript{c,*}

\textsuperscript{a} Institute for Condensed Matter Theory, University of Muenster, Wilhelm-Klemm Str. 10, D48149 Muenster, Germany
\textsuperscript{b} Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Sinaloa, Cuidad Universitaria, CP 80000, Culiacán, Sinaloa, Mexico
\textsuperscript{c} Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA

HIGHLIGHTS

- A dispersion relation is obtained and solved for surface waves on a doubly periodic Neumann surface.
- A dispersion relation is obtained and solved for surface waves on a two-dimensional randomly rough Neumann surface.
- These results are applicable to a system of a liquid in contact with a rough hard substrate.
- These are the first studies of surface waves in such systems.

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ABSTRACT

A planar surface on which a scalar wave satisfies the Neumann boundary conditions does not support a surface wave. However, a structured Neumann surface can support such a wave. By means of a Rayleigh equation for a scalar field in the region above the two-dimensional rough surface of a semi-infinite medium on which the Neumann boundary condition is satisfied, we derive the dispersion relation for surface waves on both doubly periodic and randomly rough surfaces. Dispersion curves for these waves on doubly periodic surfaces with three forms of the surface profile function are presented together with dispersion curves for surface waves on a two-dimensional randomly rough surface.

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* Corresponding author.
E-mail address: aamaradu@uci.edu (A.A. Maradudin).

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1. Introduction

In recent years interest has arisen in surface waves that propagate on impenetrable surfaces, in particular on perfectly conducting surfaces [1–18]. These surface waves cannot exist if the perfectly conducting surface on which they propagate is planar: the surface must be periodically [1–18] or randomly [1,15] rough. The interest in such waves on periodically rough perfectly conducting surfaces is due to the fact that their dispersion curves mimic those of surface plasmon polaritons on planar metallic surfaces, even though a perfect conductor has no electronic plasma that can display collective oscillations. In fact these surface waves are bound to the surface by its departure from planarity. Moreover, by varying the periodic structuring of a perfectly conducting surface, for example, by changing its period, or the heights and depths of its protuberances or indentations, or by changing the forms of these features, one can design these surface waves to possess specified properties, such as the frequency range in which they exist. Such “tuning” of the properties of these surface waves is not possible for surface plasmon polaritons on planar metallic surfaces. The existence of these waves on structured perfectly conducting surfaces has created the possibility of surface plasmon polaritons on periodically structured metallic surfaces in the gigahertz and terahertz frequency ranges, in which a metal is well represented by a perfect conductor. In these frequency ranges a surface plasmon polariton is so weakly bound to a planar metallic surface that it is in fact a surface current, not a surface wave. The existence of surface plasmon polaritons at gigahertz and terahertz frequencies is important in technological applications [19–22].

In this paper we study surface waves on a different type of impenetrable surface, namely a surface on which a scalar wave satisfies the Neumann boundary condition, i.e. a surface on which the normal derivative of the wave function of the wave vanishes. A physical situation in which this kind of surface wave can occur is a liquid on a hard substrate. It is straightforward to show that such a wave cannot exist if the surface of the substrate is planar. To see this let us denote the scalar field \( \psi(\mathbf{x}, t) \) in the region \( x_3 \geq 0 \) by \( \psi(\mathbf{x}, t) = \psi(|\mathbf{x}|, \omega) \exp(-i\omega t) \). Then the amplitude function \( \psi(|\mathbf{x}|, \omega) \) satisfies the Helmholtz equation

\[
\left[ \nabla^2 + (\omega/c)^2 \right] \psi(|\mathbf{x}|, \omega) = 0 \quad x_3 \geq 0,
\]

where \( c \) is the wave speed in this region. The solution of this equation that propagates in a wavelike fashion, in directions parallel to the plane \( x_3 = 0 \), and vanishes at \( x_3 = +\infty \) can be written as

\[
\psi(|\mathbf{x}|, \omega) = A \exp[i k_\parallel \cdot \mathbf{x}_\parallel - \beta_0(k_\parallel) x_3],
\]

where \( \mathbf{x}_\parallel = (x_1, x_2, 0) \), \( k_\parallel = (k_1, k_2, 0) \), and

\[
\beta_0(k_\parallel) = \left[ k_\parallel^2 - (\omega/c)^2 \right]^{1/2}. \quad \text{Re} \beta_0(k_\parallel) > 0, \quad \text{Im} \beta_0(k_\parallel) < 0.
\]

The dispersion relation that connects the frequency of the wave \( \omega \) with the two-dimensional wave vector \( \mathbf{k}_\parallel \) is obtained by using the solution (1.2) in the Neumann boundary condition on the surface \( x_3 = 0 \), namely

\[
\frac{\partial \psi(|\mathbf{x}|, \omega)}{\partial x_3} \bigg|_{x_3=0} = 0.
\]

In this way we obtain the condition

\[
-A \beta_0(k_\parallel) \exp[i (k_\parallel \cdot \mathbf{x}_\parallel)] = 0.
\]

In order to obtain a nontrivial solution, i.e. one for which the amplitude \( A \) is nonzero, we have to require that \( \beta_0(k_\parallel) = 0 \), which yields the dispersion relation \( \omega = c k_1 \). The field \( \psi(|\mathbf{x}|, \omega) \) in the region \( x_3 \geq 0 \) then becomes

\[
\psi(|\mathbf{x}|, \omega) = A \exp[i (k_\parallel \cdot \mathbf{x}_\parallel)].
\]

This function describes a surface skimming bulk wave that is not bound to the surface \( (\beta_0(k_\parallel) \equiv 0) \).

The wave described by Eq. (1.6) is “unstable” [23], in that even a slight change of the boundary condition on the Neumann surface converts it into a surface wave or a surface shape resonance, both of which are bound to the surface.

In this paper we demonstrate that this is the case by studying theoretically the propagation of surface waves on a structured two-dimensional Neumann surface that is doubly periodically rough or randomly rough. The corresponding problem for a one-dimensional periodically or randomly corrugated Neumann surface was studied several years ago in Refs. [24] and [25], respectively, and will not be considered here.

In the work presented here we first derive the Rayleigh equation for the scalar field in the region above a two-dimensional rough Neumann surface. We then consider a doubly periodic surface and use the Rayleigh equation to obtain the dispersion relation of the surface waves it supports, which is then solved numerically. We also obtain the dispersion relation for surface waves on a two-dimensional randomly rough Neumann surface on the basis of the small roughness approximation to the Rayleigh equation. Thus, for both types of two-dimensional surface roughness we find that a Neumann surface supports surface waves.

2. The Rayleigh equation

The physical system we consider in this work consists of an isotropic and homogeneous medium characterized by a scalar wave speed \( c \) in the region \( x_3 > \zeta(\mathbf{x}_\parallel) \), and an impenetrable medium in the region \( x_3 < \zeta(\mathbf{x}_\parallel) \). The vector \( \mathbf{x}_\parallel \) defined by
\( \mathbf{x} = (x_1, x_2, 0) \) is an arbitrary vector in the plane \( x_3 = 0 \). The surface profile function \( \zeta(\mathbf{x}_i) \) is assumed to be a single-valued function of \( \mathbf{x}_i \), that is differentiable with respect to \( x_1 \) and \( x_2 \).

We seek a solution of the scalar wave equation
\[
(\nabla^2 + (\omega/c)^2) \psi(\mathbf{x}_i|\omega) = 0
\]
(2.1)
in the region \( x_3 > \zeta(\mathbf{x}_i) \), where \( \omega \) is the frequency of the wave in this medium. A time dependence of the form \( \exp(-i\omega t) \) has been assumed for this field, but has not been indicated explicitly. We require that the solution of Eq. (2.1) satisfy the Neumann boundary condition
\[
\left[ \frac{\partial \zeta(\mathbf{x}_i)}{\partial x_1} \frac{\partial}{\partial x_1} - \frac{\partial \zeta(\mathbf{x}_i)}{\partial x_2} \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3} \right] \psi(\mathbf{x}|\omega) \bigg|_{x_3 = \zeta(\mathbf{x}_i)} = 0
\]
(2.2)
on the surface \( x_3 = \zeta(\mathbf{x}_i) \). Finally, we require that \( \psi(\mathbf{x}|\omega) \) vanish as \( x_3 \to +\infty \).

The solution of Eq. (2.1) that satisfies the boundary condition at infinity can be written in the form
\[
\psi(\mathbf{x}|\omega) = \int \frac{d^2 q_1}{(2\pi)^2} A(\mathbf{q}_i) \exp[iq_1 \cdot \mathbf{x}_1 + i\alpha_0(q_i) x_3].
\]
(2.3)
where
\[
\alpha_0(q_i) = [(\omega/c)^2 - q_i^2]^{1/2} \quad \text{Re} \alpha_0(q_i) > 0, \quad \text{Im} \alpha_0(q_i) > 0.
\]
(2.4)
When Eq. (2.3) is substituted into Eq. (2.2), we obtain as the equation for the amplitude \( A(\mathbf{q}_i) \)
\[
\int \frac{d^2 q_1}{(2\pi)^2} A(\mathbf{q}_i) \left[ -\frac{\partial \zeta(\mathbf{x}_i)}{\partial x_1} - iq_1 - \frac{\partial \zeta(\mathbf{x}_i)}{\partial x_2} - iq_2 + i\alpha_0(q_i) \right] \exp[iq_1 \cdot \mathbf{x}_1 + i\alpha_0(q_i) \zeta(\mathbf{x}_i)] = 0.
\]
(2.5)
We now introduce the representation
\[
\exp[i\gamma \zeta(\mathbf{x}_i)] = \int \frac{d^2 Q_1}{(2\pi)^2} I(\gamma|Q_i) \exp[iQ_1 \cdot \mathbf{x}_1].
\]
(2.6)
so that
\[
I(\gamma|Q_i) = \int d^2 x_1 \exp[-iQ_1 \cdot \mathbf{x}_1 + i\gamma \zeta(\mathbf{x}_i)].
\]
(2.7)
By taking the derivative of both sides of Eq. (2.6) with respect to \( x_\alpha (\alpha = 1, 2) \), we obtain
\[
\frac{\partial \zeta(\mathbf{x}_i)}{\partial x_\alpha} \exp[i\gamma \zeta(\mathbf{x}_i)] = \int \frac{d^2 Q_1}{(2\pi)^2} \frac{Q_\alpha}{\gamma} I(\gamma|Q_i) \exp[iQ_1 \cdot \mathbf{x}_1].
\]
(2.8)
On substituting Eqs. (2.6) and (2.8) with \( \gamma = \alpha_0(q_i) \) into Eq. (2.5) the latter becomes
\[
\int \frac{d^2 q_1}{(2\pi)^2} \int \frac{d^2 Q_1}{(2\pi)^2} A(\mathbf{q}_i) \frac{I(\alpha_0(q_i)|Q_i)}{\alpha_0(q_i)} \left[ -q_1 Q_1 - q_2 Q_2 + \alpha_0^2(q_i) \right] \exp i(q_1 + Q_1) \cdot \mathbf{x}_1 = 0.
\]
(2.9)
The change of variable \( q_1 + Q_1 = k_1 \) transforms Eq. (2.9) into
\[
\int \frac{d^2 k_1}{(2\pi)^2} \exp[ik_1 \cdot \mathbf{x}_1] \int \frac{d^2 q_1}{(2\pi)^2} \frac{I(\alpha_0(q_i)|k_1 - q_i)}{\alpha_0(q_i)} \left[ (\omega/c)^2 - k_1 \cdot q_i \right] A(\mathbf{q}_i) = 0.
\]
(2.10)
On equating to zero the \( k_1 \) Fourier coefficient in this equation we obtain as the equation satisfied by the amplitude \( A(\mathbf{q}_i) \)
\[
\int \frac{d^2 q_1}{(2\pi)^2} \frac{I(\alpha_0(q_i)|k_1 - q_i)}{\alpha_0(q_i)} \left[ (\omega/c)^2 - k_1 \cdot q_i \right] A(\mathbf{q}_i) = 0.
\]
(2.11)
The solvability condition for this homogeneous linear integral equation is the dispersion relation that gives the frequencies \( \omega \) for each value of the wave vector \( k_1 \). We see from Eq. (2.3) that only solutions of the dispersion relation for which the imaginary part of \( \alpha_0(q_i) \) is positive correspond to waves localized to the surface \( x_3 = \zeta(\mathbf{x}_i) \).

We now apply Eq. (2.11) to a study of surface waves on two-dimensional periodically and randomly rough surfaces.

3. A bridging

We assume here that the surface profile function \( \zeta(\mathbf{x}_i) \) is a doubly periodic function of \( \zeta(\mathbf{x}_i) \),
\[
\zeta(\mathbf{x}_1 + \mathbf{x}_i(\ell)) = \zeta(\mathbf{x}_i),
\]
(3.1)
where
\[
\mathbf{x}_i(\ell) = \ell_1 \mathbf{a}_1 + \ell_2 \mathbf{a}_2.
\]
(3.2)
In Eq. (3.2) \( a_1 \) and \( a_2 \) are the two noncollinear primitive translation vectors of a two-dimensional Bravais lattice, while \( \ell_1 \) and \( \ell_2 \) are any positive or negative integers, or zero, which we denote collectively by \( \ell \). The area of the primitive unit cell of the two-dimensional lattice defined by Eq. (3.2) is \( a_0 = |a_1 \times a_2| \).

We also introduce the lattice reciprocal to the one defined by Eq. (3.2), whose sites are given by

\[
G_i(h) = h_1 b_1 + h_2 b_2,
\]

where the primitive translation vectors \( b_1 \) and \( b_2 \) are defined by the conditions

\[
a_1 \cdot b_j = 2\pi \delta_{ij},
\]

and \( h_1 \) and \( h_2 \) are any positive or negative integers or zero that we denote collectively by \( h \).

For a surface possessing the periodicity property described by Eq. (3.1) the function \( I(x|Q_\parallel) \) becomes

\[
I(x|Q_\parallel) = \sum_{G_i} (2\pi)^2 \delta(Q_\parallel - G_\parallel) \hat{I}(x|G_\parallel),
\]

where

\[
\hat{I}(x|G_i) = \frac{1}{a_c} \int_{a_c} d^2x \exp(-iG_i \cdot x) \exp(i\omega x)\zeta(x).
\]

In obtaining this expression we have used the result

\[
\sum_\ell \exp[-iQ_\parallel \cdot x(\ell)] = \frac{(2\pi)^2}{a_c} \sum_{G_i} \delta(Q_\parallel - G_\parallel).
\]

In order that the field in the region \( x_3 > \zeta(x) \) satisfy the Floquet–Bloch condition

\[
\psi(x + x_i(\ell), x_3|\omega) = \exp(iQ_i \cdot x)\psi(x, x_3|\omega),
\]

we write the amplitude \( A(q_\parallel) \) in the form

\[
A(q_\parallel) = \sum_{G_i} (2\pi)^2 \delta(q_\parallel - k_\parallel - G_\parallel) a_{k_\parallel}(G_\parallel),
\]

where \( k_\parallel \) is the two-dimensional wave vector of the surface wave.

When the results given by Eqs. (3.5) and (3.9) are substituted into Eq. (2.11) we obtain as the equation for the coefficients \( \{a_{k_\parallel}(G_\parallel)\} \)

\[
\sum_{G_i} \hat{I}(x|G_i) \delta(G_i - G_\parallel) \frac{[(\omega/c)^2 - (k_\parallel + G_\parallel) \cdot (k_\parallel + G_\parallel')]}{a_0(|k_\parallel + G_\parallel|)} a_{k_\parallel'}(G_\parallel') = 0.
\]

The dispersion relation for surface waves on a bigrating on which the Neumann boundary condition is imposed is then obtained by equating to zero the determinant of the matrix of coefficients in Eq. (3.10).

The solutions of this equation are even functions of \( k_\parallel \), \( \omega_0(-k_\parallel) = \omega_0(k_\parallel) \), where \( s \) labels the solutions for a given value of \( k_\parallel \) in the order of increasing magnitude. They are also periodic functions of \( k_\parallel \) with the periodicity of the reciprocal lattice, \( \omega_0(k_\parallel + G_\parallel) = \omega_0(k_\parallel) \). The solutions can therefore be sought for values of \( k_\parallel \) inside the first Brillouin zone of the bigrating, and inside the nonradiative region of \( \omega \) and \( k_\parallel \) values, defined by \(|k_\parallel| > (\omega/c)\).

In the present work we have calculated the solutions of the dispersion relation obtained from Eq. (3.10) for three forms of the surface profile function \( \zeta(x) \). We consider them in turn.

### 3.1. A square lattice of hemiellipsoids

In our first example the surface profile function is represented by a square array of hemiellipsoids on an otherwise planar Neumann surface. The primitive translation vectors of the square lattice are

\[
a_1 = a(1, 0), \quad a_2 = a(0, 1).
\]

The primitive translation vectors of the corresponding reciprocal lattice are

\[
b_1 = \frac{2\pi}{a}(1, 0), \quad b_2 = \frac{2\pi}{a}(0, 1).
\]

The surface profile function describing a square lattice of hemiellipsoids or radius \( R \) (<\( a \)) and height \( HR \) can be written as

\[
\zeta(x) = \sum_{\ell} s(x_\parallel - x_\parallel(\ell)),
\]

where

\[
s(x_\parallel) = \begin{cases} H(R^2 - x_\parallel^2)^{\frac{3}{2}} & |x_\parallel| < R \\ 0 & |x_\parallel| > R. \end{cases}
\]
Because each hemiellipsoid has circular symmetry the dispersion relation satisfies the relation
\[ \omega_i (\mathbf{S} \mathbf{k}_i) = \omega_i (\mathbf{k}_i), \]  
(3.15)
where \( \mathbf{S} \) is a \( 2 \times 2 \) real orthogonal matrix representative of any of the point group operations that leave the square lattice invariant. In the present case they constitute the point group \( C_{4v} \). The property expressed by Eq. (3.15) has the consequence that all of the independent solutions of the dispersion relation are obtained if the wave vector \( \mathbf{k}_i \) is restricted to the irreducible element of the two-dimensional first Brillouin zone. This is the region of the Brillouin zone that generates the entire zone when transformed by the application of the operations of the point group \( C_{4v} \) to it.

The function \( I(\gamma | \mathbf{G}_i) \) for the surface profile function defined by Eqs. (3.13)–(3.14) is given by [26]
\[
I(\gamma | \mathbf{G}_i) = 1 + \frac{2\pi R^2}{a^2} \sum_{n=1}^{\infty} \frac{(iyHR)^n}{(n+2)!} \mathbf{G}_i = 0
\]
(3.16a)
\[
= \frac{2\pi R^2}{a^2} \sum_{n=1}^{\infty} \frac{(iyHR)^n}{n!} \frac{2^n I(\frac{\gamma}{2}) + 1}{(\mathbf{G}_i R)^{\frac{n}{2}+1}} J_{\frac{n}{2}+1}(\mathbf{G}_i R) \quad \mathbf{G}_i \neq 0,
\]
(3.16b)
where \( J_n(x) \) is a Bessel function of the first kind of order \( \nu \), and \( I_n(x) \) is the gamma function. For the values of the parameters used in the numerical calculations based on the results obtained in this section it was necessary to include only the first few (\( \approx 15 \)) terms in these rapidly convergent series.

To solve the dispersion relation obtained from Eq. (3.10) the infinite sum over \( \mathbf{G}_i \) has to be truncated. This was done by restricting the reciprocal-lattice vectors \( \mathbf{G}_i(h) = h_1 \mathbf{b}_1 + h_2 \mathbf{b}_2 \) and \( \mathbf{G}_i(h) = h_1' \mathbf{b}_1 + h_2' \mathbf{b}_2 \) to those that satisfied the conditions
\[
(h_1^2 + h_2^2)^{\frac{1}{2}} \leq N_{\text{max}} \quad \text{and} \quad (h_1'^2 + h_2'^2)^{\frac{1}{2}} \leq N_{\text{max}}.
\]
The convergence of a solution was tested by increasing \( N_{\text{max}} \) systematically until it stopped changing.

The determination of the dispersion curves was based on the search for real zeros of a real-valued determinant. For a value of \( \mathbf{k}_i \) inside or on the boundary of the irreducible element of the first Brillouin zone the frequency \( \omega \) was increased systematically in the interval \( 0 \leq \omega \leq \epsilon k_i \) and changes in the sign of the determinant were sought. The frequencies at which this occurred were labeled in the order of increasing magnitude. This collection constitutes the different branches of the dispersion curve.

In Fig. 1(a) we present dispersion curves for wave vectors \( \mathbf{k}_i \) on the boundary of the irreducible element of the first surface Brillouin zone. This element is displayed in the inset to this figure. Note that these curves are plotted as functions of \( k_i = |\mathbf{k}_i| \). This way of plotting the dispersion curves gives rise to the discontinuity of their slope in the vicinity of the \( X \) point. The values of the parameters assumed in obtaining this figure were \( R/a = 0.375 \) and (a) \( H = 0.5 \), \( H = 1 \); (b) \( H = -0.5 \), \( H = -1 \). In all of these calculations \( N_{\text{max}} = 10 \). The surface thus consists of a square lattice of hemiellipsoidal protuberances (Fig. 1(a)) or of hemiellipsoidal indentations (“dimples”) (Fig. 1(b)). For the values of the parameters defining the surface each dispersion curve consists of only a single branch within the nonradiative region of \( \omega \) and \( \mathbf{k}_i \) values. All frequencies above the maximum frequency of the branch constitute a stop band. Each dispersion curve displays the phenomenon of wave slowing as \( \mathbf{k}_i \) approaches the boundaries of the Brillouin zone, i.e. the phase and group velocities of the surface wave decrease. Each curve possesses a zero slope at the high symmetry points on the zone boundary. From a comparison of Figs. 1(a) and (b) it is seen that increasing \( |H| \) depresses the dispersion curves for lattices of protuberances and indentations, but more strongly for the latter type of surface than for the former.

It is an open question as to whether increasing the magnitude of \( H \) further will lead to a second, higher frequency, branch of the dispersion curve entering the nonradiative region. Numerical instabilities in the present calculations for values of \( |H| \) larger than unity have prevented us from answering this question.

3.2. An orthogonal superposition of two sinusoidal gratings

The second form of the surface profile function we consider is given by
\[
\zeta (\mathbf{x}_i) = \zeta_0 \left( \cos \frac{2\pi x_1}{a} + \cos \frac{2\pi x_2}{a} \right).
\]
(3.17)
For this profile function it suffices to calculate dispersion curves only for negative values of \( \zeta_0 \), because a change of the sign of \( \zeta_0 \) corresponds to a shift of the origin of coordinates by \( (a/2, a/2) \), which does not change the dispersion curve. The primitive translation vectors of the square lattice defined by this surface profile function and of the lattice reciprocal to it, are given by Eqs. (3.11) and (3.12), respectively, and the symmetry point group of this surface is \( C_{4v} \).

The function \( I(\gamma | \mathbf{G}_i) \) for this choice of surface profile function can be written
\[
I(\gamma | \mathbf{G}_i) = i^{m+n} J_m(\gamma \zeta_0) J_n(\gamma \zeta_0),
\]
(3.18)
where \( J_m(x) \) is a Bessel function of the first kind of order \( m \). The integers \( m, n = 0, \pm 1, \pm 2, \ldots \) are defined by
\[
\mathbf{G}_i = \frac{2\pi}{a} (m, n, 0).
\]
(3.19)
Fig. 1. Dispersion curves for surface waves on a square lattice of hemiellipsoids on an otherwise planar Neumann surface. The single branch of the dispersion curve in the nonradiative region of $\omega$ and $k_a$ values is plotted as a function of $k_a$ along the boundary of the irreducible element of the first surface Brillouin zone. The dotted line represents the dispersion curve $\omega = ck_a$. The values of the parameters assumed in obtaining these results are: (a) $R/a = 0.375$, and $H = 0.5 (- - - - -)$, $H = 1 (- - - - -)$; (b) $H = -0.5 (- - - - -)$, $H = -1 (- - - - -)$. $N_{\text{max}} = 10$ in all of these calculations. The insets from left to right depict the irreducible element of the first surface Brillouin zone, an enlargement of the band structure in the vicinity of the $\bar{X}$ point, and an enlargement of the band structure in the vicinity of the $\bar{M}$ point.

Fig. 2. Dispersion curves for surface waves on a Neumann surface defined by the surface profile function given by Eq. (3.17). The values of the parameters assumed in obtaining these results are $\zeta_0/a = -0.1(- - - - -)$, $\zeta_0/a = -0.2(- - - - -)$. $N_{\text{max}} = 12$.

The dispersion relation for this surface, obtained from Eq. (3.10) is solved just as in the case of the surface defined by Eqs. (3.13)-(3.14).

We plot the dispersion curve obtained in this way in Fig. 2 for the values of the parameters defining the surface profile function given by $\zeta_0/a = -0.1$, $\zeta_0/a = -0.2$, and $N_{\text{max}} = 12$. It consists of a single branch in the nonradiative region of $\omega$.
and $k_\parallel$ values. It displays wave slowing. Increasing $|\xi_0/a|$ depresses the dispersion curve in frequency, causing it to depart from the dispersion curve $\omega = c k_\parallel$ into the nonradiative region at smaller values of $k_\parallel$.

### 3.3. An orthogonal superposition of two symmetric sawtooth gratings

In our third example the doubly periodic surface is an orthogonal superposition of two identical symmetric sawtooth gratings. The surface profile function $\zeta(x)$ has the form given by Eq. (3.13), where the function $s(x)$ is now defined by

$$s(x) = H \left(1 - \frac{2|x_1|}{a}\right) + H \left(1 - \frac{2|x_2|}{a}\right); \quad \frac{a}{2} < x_1 < \frac{a}{2}, \frac{a}{2} < x_2 < \frac{a}{2}. \tag{3.20}$$

For this surface profile function it is sufficient to calculate dispersion curves only for positive values of $H$, because a change of the sign of $H$ corresponds to a shift of the origin of coordinates by $(a/2, a/2)$, followed by a vertical displacement of the surface by $2H$, which does not change the dispersion curve. The primitive translation vectors of the square lattice defined by this surface profile function, and of the lattice reciprocal to it, are given by Eqs. (3.11) and (3.12), respectively, and the symmetry point group of this surface is $C_{4v}$.

The function $\hat{I}(\gamma|G_{ij})$ for this surface profile function is

$$\hat{I}(\gamma|G_{ij}) = 4 \exp(i\gamma H) \frac{(\gamma H)^2}{[(\gamma H)^2 - (m\pi)^2][(\gamma H)^2 - (n\pi)^2]} j(m) j(n), \tag{3.21}$$

where

$$j(m) = \begin{cases} \sin \frac{1}{2} \gamma H & m \text{ even} \quad (a) \\ -i \cos \frac{1}{2} \gamma H & m \text{ odd.} \quad (b) \end{cases} \tag{3.22}$$

The integers $m, n = 0, \pm 1, \pm 2, \ldots$ are defined by Eq. (3.19).

The dispersion curve obtained from the solvability condition for Eq. (3.10) is plotted in Fig. 3 for the values of the parameters defining the surface profile function given by $H/a = 0.2$, $N_{\text{max}} = 12$ and $H/a = 0.4$, $N_{\text{max}} = 4$. It consists of a single branch in the nonradiative region of $\omega$ and $k_\parallel$ values for both values of $H/a$, and displays wave slowing. Increasing $H$ depresses the dispersion curve toward lower frequencies.

We believe that the small value of $N_{\text{max}} = 4$ used in obtaining the dispersion curve when $H/a = 4$ is due to the nonanalytic nature of the surface profile function (3.20). It is known that the Rayleigh hypothesis is invalid for a one-dimensional periodic surface defined by a nonanalytic profile function [27]. It is assumed, without proof, that the same result holds for a doubly periodic surface defined by a nonanalytic surface profile function. When a one- or two-dimensional nonanalytic periodic surface profile function is expanded in a finite number of plane waves, it is an analytic function of the coordinates, for which the Rayleigh hypothesis is valid when its amplitude to period ratio is sufficiently small. However, as more and more plane waves are included in the expansion of the surface profile function, i.e. when $N_{\text{max}}$ is increased, a point is reached where the nonanalytic nature of the surface profile function begins to manifest itself, and the Rayleigh hypothesis breaks down. A further increase in $N_{\text{max}}$ simply worsens the result. Thus the convergence of the expansion of the scalar field in plane waves has an asymptotic character. In the calculations based on the profile function (3.20) the optimal value of $N_{\text{max}}$ is 4 for the rough surface with $H/a = 0.4$, while it is $N_{\text{max}} = 12$ for the smoother surface with $H/a = 0.2$.

Similar considerations apply to the results presented in Fig. 1 for another surface defined by a nonanalytic profile function.
4. A randomly rough surface

We now assume that the surface profile function $\zeta(x_1)$, in addition to being a single-valued function of $x_1$ and differentiable with respect to $x_1$ and $x_2$, constitutes a stationary, zero-mean, isotropic, Gaussian random process defined by

$$
\langle \zeta(x_1) \zeta(x_1') \rangle = \delta^2 W(|\mathbf{x}_1 - \mathbf{x}_1'|).
$$

(4.1)

In this equation the angle brackets denote an average over the ensemble of realizations of the surface profile function, while $\delta = (\langle \zeta^2(x_1) \rangle)^{1/2}$ is the rms height of the surface.

In what follows we will need the Fourier integral representation of $\zeta(x_1)$,

$$
\zeta(x_1) = \int \frac{d^2 \mathbf{Q}_1}{(2\pi)^2} \hat{\zeta}(\mathbf{Q}_1) \exp(i \mathbf{Q}_1 \cdot \mathbf{x}_1).
$$

(4.2)

The Fourier coefficient $\hat{\zeta}(\mathbf{Q}_1)$ is also a zero-mean Gaussian random process that is defined by

$$
\langle \hat{\zeta}(\mathbf{Q}_1) \hat{\zeta}(\mathbf{Q}_1') \rangle = (2\pi)^2 \delta(\mathbf{Q}_1 + \mathbf{Q}_1') \delta^2 g(||\mathbf{Q}_1||).
$$

(4.3)

The function $g(||\mathbf{Q}_1||)$ entering this equation is the power spectrum of the surface roughness, and is defined by

$$
g(||\mathbf{Q}_1||) = \int d^2 x_1 W(|\mathbf{x}_1|) \exp(-i \mathbf{Q}_1 \cdot \mathbf{x}_1).
$$

(4.4)

To obtain the dispersion relation for surface waves on a randomly rough Neumann surface we will use the small roughness approximation. This consists of expanding the function $I(\alpha_0(q_0)||k|| - q_0)$ in Eq. (2.11) in powers of the surface profile function and retaining only the first two terms:

$$
I(\alpha_0(q_0)||k|| - q_0) = (2\pi)^2 \delta(k|| - q_0) + i\alpha_0(q_0) \hat{\zeta}(k|| - q_0) + O(\zeta^2).
$$

(4.5)

Eq. (2.11) can then be rewritten in the form

$$
\alpha_0(k||)A(k||) = \int \frac{d^2 q_{||}}{(2\pi)^2} V(k|| |q||)A(q||),
$$

(4.6)

where

$$
V(k|| |q||) = -i[\omega/c^2 - k|| \cdot q||] \hat{\zeta}(k|| - q||).
$$

(4.7)

The surface profile function entering Eq. (4.7) is a random process. Consequently the solution $A(k||)$ of Eq. (4.6) is a random process. Just as $\zeta(x_1)$ is defined by the moments of its probability density function, so can $A(k||)$ be defined by the moments of its probability density function. Of these a particularly important one is the first moment $\langle A(k||) \rangle$, which describes the propagation of the mean wave across the randomly rough surface.

To obtain the equation satisfied by $\langle A(k||) \rangle$ we introduce the smoothing operator $P$ that averages every function to which it is applied over the ensemble of realizations of the surface profile function [28]. We also introduce the complementary operator $Q = 1 - P$, that produces the fluctuating part of every function on which it acts. On applying these operators to Eq. (4.6) we obtain the pair of equations

$$
\alpha_0(k||)PA(k||) = \int \frac{d^2 q_{||}}{(2\pi)^2} PV(k|| |q||)[PA(q||) + QA(q||)]
$$

(4.8)

$$
\alpha_0(q||)QA(q||) = \int \frac{d^2 r_{||}}{(2\pi)^2} QV(q|| |r||)[PA(r||) + QA(r||)].
$$

(4.9)

When we use the results that $PV(k|| |q||) = 0$, because $\zeta(x_1)$ is a zero-mean random process, and that $QA(r||)$ is of order $\zeta(x_1)$, Eqs. (4.8)–(4.9) simplify to

$$
\alpha_0(k||)PA(k||) = \int \frac{d^2 q_{||}}{(2\pi)^2} PV(k|| |q||)QA(q||)
$$

(4.10)

$$
\alpha_0(q||)QA(q||) = \int \frac{d^2 r_{||}}{(2\pi)^2} V(q|| |r||)PA(r||).
$$

(4.11)

On combining Eqs. (4.10) and (4.11) we obtain as the equation satisfied by the mean amplitude $\langle A(k||) \rangle$

$$
\alpha_0(k||)\langle A(k||) \rangle = \int \frac{d^2 q_{||}}{(2\pi)^2} \int \frac{d^2 r_{||}}{(2\pi)^2} \frac{V(k|| |q||)V(q|| |r||)}{\alpha_0(q||)} \langle A(r||) \rangle.
$$

(4.12)
The result that
\[(V(k_i|q_i)V(q_i|r_j)) = (2\pi)^2 \delta(k_i - r_j) \delta^2 g(|k_i - q_i|)[(\omega/c)^2 - k_i \cdot q_i]^2,\]  
which follows from Eqs. (4.3) and (4.7), reduces Eq. (4.12) to
\[\alpha_0(k_1) \langle A(k_1) \rangle = -\delta^2 \int \frac{d^2q_\parallel}{(2\pi)^2} g(|k_1 - q_\parallel|) \frac{[(\omega/c)^2 - k_i \cdot q_i]^2}{\alpha_0(q_\parallel)} \langle A(k_1) \rangle.\]  
The dispersion relation for surface waves on a randomly rough two-dimensional Neumann surface is therefore
\[\alpha_0(k_1) = -\delta^2 \int \frac{d^2q_\parallel}{(2\pi)^2} g(|k_1 - q_\parallel|) \frac{[(\omega/c)^2 - k_i \cdot q_i]^2}{\alpha_0(q_\parallel)}.\]  
The power spectrum \(g(|k_i - q_\parallel|)\) can be written in the form
\[g(k_1 - q_\parallel) = \sum_{m=-\infty}^{\infty} g_m(k_\parallel|q_\parallel) \exp[-im(\phi_k - \phi_q)].\]  
where
\[g_m(k_\parallel|q_\parallel) = 2\pi \int_0^\infty dx_i x_i W(|k_\parallel|) j_m(k_\parallel x_i) j_m(q_\parallel x_\parallel)\]
\[= g_{-m}(k_\parallel|q_\parallel),\]  
\(j_m(x)\) is a Bessel function of the first kind of order \(m\), and \(\phi_k\) and \(\phi_q\) are the azimuthal angles of the vectors \(k_i\) and \(q_i\), respectively. When Eq. (4.16) is substituted into Eq. (4.15) and the angular integration is carried out, the latter equation becomes
\[\alpha_0(k_1) = -\frac{\delta^2}{2\pi} \int_0^\infty dq_\parallel \frac{q_\parallel}{\alpha_0(q_\parallel)} [A_0(k_\parallel|q_\parallel) + B_1(k_\parallel|q_\parallel) + C_2(k_\parallel|q_\parallel)].\]  
where
\[A = \left(\frac{\omega}{c}\right)^4 + \frac{1}{2} k_\parallel^2 q_\parallel^2\]  
\[B = -2 \left(\frac{\omega}{c}\right)^3 k_\parallel q_\parallel\]  
\[C = \frac{1}{2} k_\parallel^2 q_\parallel.\]  
If we now take Eq. (2.4) into account, we can rewrite Eq. (4.18) as
\[\alpha_0(k_1) = -\frac{\delta^2}{2\pi} \int_0^{\omega/c} dq_\parallel \frac{q_\parallel}{[(\omega/c)^2 - q_\parallel^2]^2} [A_0(k_\parallel|q_\parallel) + B_1(k_\parallel|q_\parallel) + C_2(k_\parallel|q_\parallel)] + i \frac{\delta^2}{2\pi} \int_0^{\omega/c} dq_\parallel \frac{q_\parallel}{[q_\parallel^2 - (\omega/c)^2]^2} [A_0(k_\parallel|q_\parallel) + B_1(k_\parallel|q_\parallel) + C_2(k_\parallel|q_\parallel)].\]  
We now make the Ansatz
\[\frac{\omega^2}{c^2} = k_\parallel^2 - \delta^4 \Delta^2(k_\parallel).\]  
It then follows from Eq. (2.4) that
\[\alpha_0(k_1) = i\delta^2 \Delta(k_\parallel, \omega),\]  
where
\[\Delta(k_\parallel, \omega) = \frac{1}{2\pi} \int_0^{\omega/c} dq_\parallel \frac{q_\parallel}{[q_\parallel^2 - (\omega/c)^2]^2} [A_0(k_\parallel|q_\parallel) + B_0(k_\parallel|q_\parallel) + C_2(k_\parallel|q_\parallel)] + i \frac{1}{2\pi} \int_0^{\omega/c} dq_\parallel \frac{q_\parallel}{[(\omega/c)^2 - q_\parallel^2]^2} [A_0(k_\parallel|q_\parallel) + B_1(k_\parallel|q_\parallel) + C_2(k_\parallel|q_\parallel)].\]
From Eqs. (4.22) and (4.24) we obtain

\[ \Delta(k_l, \omega) \cong \Delta(k_{l1}, ck_{l1}) = \Delta_1(k_{l1}) + i \Delta_2(k_{l1}), \] (4.24)

where

\[
\Delta_1(k_{l1}) = \frac{1}{2\pi} \int_{k_{l1}}^{\infty} dq_{l1} \frac{q_{l1} \left( \frac{1}{2} k_{l1}^2 q_{l1}^2 + k_{l1}^4 \right) g_0(k_{l1}|q_{l1})}{(q_{l1}^2 - k_{l1}^2)^{3/2}} \left[ \left( \frac{1}{2} k_{l1}^2 q_{l1}^2 + k_{l1}^4 \right) g_0(k_{l1}|q_{l1}) - 2k_{l1}^3 q_{l1} g_1(k_{l1}|q_{l1}) + \frac{1}{2} k_{l1}^2 q_{l1}^2 g_2(k_{l1}|q_{l1}) \right] \]

(4.25a)

\[
\Delta_2(k_{l1}) = \frac{1}{2\pi} \int_{0}^{k_{l1}} dq_{l1} \frac{q_{l1} \left( \frac{1}{2} k_{l1}^2 q_{l1}^2 + k_{l1}^4 \right) g_0(k_{l1}|q_{l1})}{(k_{l1}^2 - q_{l1}^2)^{3/2}} \left[ \left( \frac{1}{2} k_{l1}^2 q_{l1}^2 + k_{l1}^4 \right) g_0(k_{l1}|q_{l1}) - 2k_{l1}^3 q_{l1} g_1(k_{l1}|q_{l1}) + \frac{1}{2} k_{l1}^2 q_{l1}^2 g_2(k_{l1}|q_{l1}) \right]. \]

(4.25b)

From Eqs. (4.22) and (4.24) we obtain

\[ \alpha_0(k_{l1}) = \delta^2 \left[ -\Delta_2(k_{l1}) + i \Delta_1(k_{l1}) \right]. \] (4.26)

Since from Eq. (2.3) we see that the imaginary part of \( \alpha_0(q_{l}) \) must be positive for the wave to be bound to the surface, it follows from Eq. (4.26) that \( \Delta_1(k_{l1}) \) must be positive.

In obtaining numerical results for \( \Delta_1(k_{l1}) \) and \( \Delta_2(k_{l1}) \) we assume that the normalized surface height autocorrelation function \( W(|x_{l1}|) \) has the Gaussian form

\[ W(|x_{l1}|) = \exp(-x_{l1}^2/a^2). \] (4.27)

The coefficient function \( g_m(k_{l1}|q_{l1}) \), Eq. (4.17), in this case is given by

\[ g_m(k_{l1}|q_{l1}) = \pi a^2 \exp[-(k_{l1}^2 + q_{l1}^2)a^2/4] I_m(k_{l1}a^2/2), \] (4.28)

where \( I_m(x) \) is a modified Bessel function of the first kind of order \( m \). The expressions (4.25a) and (4.25b) for \( \Delta_1(k_{l1}) \) and \( \Delta_2(k_{l1}) \) become

\[
\Delta_1(k_{l1}) = \frac{a^2}{2} \exp(-a^2 k_{l1}^2/4) \int_{k_{l1}}^{\infty} dq_{l1} \left[ \frac{1}{(q_{l1}^2 - k_{l1}^2)^{3/2}} \left( \frac{1}{2} k_{l1}^2 q_{l1}^2 + k_{l1}^4 \right) \right] g_0(k_{l1}|q_{l1}) \left[ 2k_{l1}^3 q_{l1} g_1(k_{l1}|q_{l1}) + \frac{1}{2} k_{l1}^2 q_{l1}^2 g_2(k_{l1}|q_{l1}) \right] \]

(4.29a)

\[
\Delta_2(k_{l1}) = \frac{a^2}{2} \exp(-a^2 k_{l1}^2/4) \int_{0}^{k_{l1}} dq_{l1} \left[ \frac{1}{(k_{l1}^2 - q_{l1}^2)^{3/2}} \left( \frac{1}{2} k_{l1}^2 q_{l1}^2 + k_{l1}^4 \right) \right] g_0(k_{l1}|q_{l1}) \left[ 2k_{l1}^3 q_{l1} g_1(k_{l1}|q_{l1}) + \frac{1}{2} k_{l1}^2 q_{l1}^2 g_2(k_{l1}|q_{l1}) \right]. \]

(4.29b)

If we introduce the definition \( x = k_{l1} a \), and make the changes of variables \( q_{l1} = (x/a) \cosh \theta \) in Eq. (4.29a) and \( q_{l1} = (x/a) \sin \theta \) in Eq. (4.29b), we find that

\[ \Delta_{1,2}(k_{l1}) = \frac{x^2}{2a^3} d_{1,2}(x), \] (4.30)

where

\[
d_1(x) = \exp(-x^2/4) \int_{0}^{\infty} d\theta \cos \theta \exp[-(x^2/4) \cos^2 \theta] \left[ \left( \frac{1}{2} \cosh^2 \theta + 1 \right) I_0 \left( \frac{x^2}{2} \cosh \theta \right) - 2 \cos \theta I_1 \left( \frac{x^2}{2} \cosh \theta \right) + \frac{1}{2} \cosh^2 \theta I_2 \left( \frac{x^2}{2} \cosh \theta \right) \right] \]

(4.31a)

\[
d_2(x) = \exp(-x^2/4) \int_{0}^{\frac{\pi}{2}} d\theta \sin \theta \exp[-(x^2/4) \sin^2 \theta] \left[ \left( \frac{1}{2} \sin^2 \theta + 1 \right) I_0 \left( \frac{x^2}{2} \sin \theta \right) - 2 \sin \theta I_1 \left( \frac{x^2}{2} \sin \theta \right) + \frac{1}{2} \sin^2 \theta I_2 \left( \frac{x^2}{2} \sin \theta \right) \right]. \]

(4.31b)

In the long wavelength limit \( x \to 0 \) the universal functions \( d_1(x) \) and \( d_2(x) \) take the forms [4]

\[ d_1(x) = \frac{\sqrt{\pi}}{2} \left( \frac{2}{x^3} - \frac{3}{2x} + O(x) \right) \] (4.32a)

\[ d_2(x) = \frac{4}{3} - \frac{9}{10} x^2 + O(x^4). \] (4.32b)
If we combine the results given by Eqs. (4.21), (4.24), and (4.30), we find that the dispersion relation for surface waves on a two-dimensional, randomly rough, Neumann surface can be written in the form

$$\omega(k) = ck \left[ 1 - \frac{\delta}{a} \omega_1(x) - i \left( \frac{\delta}{a} \right)^4 \omega_2(x) \right],$$

(4.33)

where

$$\omega_1(x) = \frac{x^8}{8} \left[ d_1^2(x) - d_2^2(x) \right] = \frac{\pi}{8} \left[ x^2 - \frac{3}{2} x^4 + O(x^6) \right] x \to 0$$

(4.34a)

$$\omega_2(x) = \frac{x^8}{4} d_1(x) d_2(x) = \frac{\sqrt{\pi}}{3} x^5 \left[ 1 - \frac{57}{40} x^2 + O(x^4) \right] x \to 0.$$  

(4.34b)

Thus, in the long wavelength limit the surface wave dispersion relation is

$$\omega(k) = ck \left[ 1 - \frac{\pi}{8} \left( \frac{\delta}{a} \right)^4 x^2 \right] - i c k \frac{\sqrt{\pi}}{3} \left( \frac{\delta}{a} \right)^4 x^5 x \to 0.$$  

(4.35)

The function $\alpha_0(k)$ obtained from Eqs. (4.26), (4.30), and (4.32) is given by

$$\alpha_0(k) = \frac{\delta^2}{2a^3} x^5 \left[ -d_2(x) + id_1(x) \right] = \frac{\delta^2}{2a^3} \left[ -\frac{4}{3} x^5 + i \sqrt{\pi} x^3 \right] x \to 0.$$  

(4.36)

In Fig. 4 we have plotted $d_1(x)$ and $d_2(x)$ as functions of $x$, while the functions $\omega_1(x)$ and $\omega_2(x)$ are plotted in Fig. 5.

The functions $d_1(x)$ and $d_2(x)$ are seen to be positive for all values of $x$. One of the consequences of these results is that the inverse decay length of the wave into the vacuum, $Im \alpha_0(k)$, is always positive. Thus the wave is bound to the surface for all values of $x = k_1 a$. In the long wavelength limit $Im \alpha_0(k)$ is proportional to $k_1^2$ (Eq. (4.36)). This wave is therefore weakly bound to the surface in this limit, but it is bound nonetheless.
A second consequence of the positivity of $d_1(x)$ and $d_2(x)$ is that $\text{Im} \omega_0(k) = -ck_0(\delta/a)^4(x^8/4)\text{d}_1(x)\text{d}_2(x)$ is negative for all $x$. This means that the surface wave is attenuated as it propagates along the randomly rough surface for all values of $x$. In the long wavelength limit $\text{Im} \omega_0(k)$ is proportional to $k^2$ (Eqs. (4.33), (4.34b)) which, in view of Eq. (4.33) means that it is proportional to the sixth power of its frequency. The explanation for this dependence begins with the observation that the frequency dependent of Rayleigh scattering is $\omega^4$ [15]. We have included the resulting dispersion curve for completeness.

We also note that despite the difference between the physical systems studied, and the difference between the equations to be solved, the dispersion relation for a surface wave on a two-dimensional randomly rough Neumann surface turns out to be the same as the dispersion relation for surface electromagnetic waves on a two-dimensional randomly rough perfectly conducting surface in contact with vacuum [15]. We have included the resulting dispersion curve for completeness.

We conclude this section by noting that the right-hand side of Eq. (4.15) is proportional to $\delta^2$. It might be thought that including the next term in the expansion of $I(\omega_0(q))|k_\parallel - q_\parallel|$ given by Eq. (4.5), namely $-(1/2)\alpha_0^2(q_\parallel)\xi^{(2)}(k_\parallel - q_\parallel)$, where

$$\xi^{(2)}(Q_\parallel) = \int d^2\parallel x_\parallel \parallel^2 x_\parallel \exp(-iQ_\parallel \cdot x_\parallel),$$

would add another term proportional to $\delta^2$ to the right-hand side of Eq. (4.15). In fact, the inclusion of this term in Eq. (4.5) has the result that the left-hand side of Eq. (4.15) becomes $[1 - (1/2)\alpha_0^2(k_\parallel)]\omega_0(k_\parallel)$. The presence of the term $-(1/2)\alpha_0^2(k_\parallel)$ in this expression leads to a correction to Eq. (4.15) for $\omega_0(k_\parallel)$ of $\mathcal{O}(\delta^4)$, which we have neglected.

5. Conclusions

The results presented here have been obtained for a simple system that demonstrates how the structuring of a surface can make it support a surface wave that does not exist in the absence of the structuring. The structuring can be periodic or it can be random. The resulting modes are dispersive because of the presence of a characteristic length in the problem: the lattice parameter in the case of the bichromatic, and the transverse correlation length in the case of the randomly rough surface. They display wave slowing. As the height of the protuberances, or depths of indentations of doubly periodic surfaces and the rms height of a randomly rough surface is increased, the dispersion curve of the corresponding surface waves bends away from the dispersion curve $\omega = c_\parallel$ into the nonradiative region of $\omega$ and $k_\parallel$ values at smaller and smaller values of $k_\parallel$. The frequency range within which these waves exist shrinks correspondingly. Increasing the period of the bichromatic or increasing the height of the protuberances or the depth of the indentations, or decreasing the value of $\delta/a$ for the randomly rough surface, has the opposite effect: the surface wave dispersion curve moves closer to the dispersion curve $\omega = c_\parallel$. In general, the dispersion curves of these surface waves can be modified in desirable ways by suitable choices of the parameters that define the roughness of the doubly periodic or randomly rough surface.

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