Recovery of inclusion separations in strongly heterogeneous composites from effective property measurements

Chris Orum, Elena Cherkaev, Kenneth M. Golden

University of Utah, Department of Mathematics, 155 South 1400 East, JWB 233, Salt Lake City UT 84112-0090 USA

An effective property of a composite material consisting of inclusions within a host matrix depends on the geometry and connectedness of the inclusions. This dependence may be quite strong if the constituents have highly contrasting properties. Here we consider the inverse problem of using effective property data to obtain information on the geometry of the microstructure. While previous work has been devoted to recovering the volume fractions of the constituents, our focus is on their connectedness—a key feature in critical behavior and phase transitions. We solve exactly a reduced inverse spectral problem by bounding the volume fraction of the constituents, an inclusion separation parameter, and the spectral gap of a self-adjoint operator that depends on the geometry of the composite. We present a new algorithm based on the Möbius transformation structure of the forward bounds whose output is a set of algebraic curves in parameter space bounding regions of admissible parameter values. These results advance the development of techniques for characterizing the microstructure of composite materials. As an example, we obtain inverse bounds on the volume fraction and separation of the brine inclusions in sea ice from measurements of its effective complex permittivity.

1. Introduction

We consider the problem of recovering information on the microgeometry of heterogeneous two phase media from measurements of its effective electromagnetic properties. In the case of highly contrasting phases, as addressed herein, the effective property can depend quite strongly on the connectedness of one of the phases. This may be seen, for example, in the case that the effective property is effective conductivity and one phase is a good conductor and the other is a good insulator.

Our analysis of this inverse problem is intimately connected with the theory of forward bounds on the effective properties of composite media. Landmarks in the forward theory include the arithmetic and harmonic mean bounds (Wiener 1912), the bounds of Hashin & Shtrikman (1962), and the improved translation bounds (Cherkaev 2000; Milton 2002). The classical derivation of these bounds relies on energy variational principles that are not readily extendible to the interaction of
composites with wave fields. If the wavelength of the electromagnetic field is long compared to the scale of the microstructure then material parameters can assume complex values. Cherkaev & Gibiansky (1994) extended the variationally derived bounds to complex parameters. See also (Cherkaev 2000; Milton 2002).

An alternative approach pioneered by Bergman (1980) and Milton (1980) and developed further by Golden & Papanicolaou (1983) uses analytic continuation for representing and bounding effective properties in the complex case. Analyticity of \( m(h) \), where \( m = \sigma^*/\sigma_2 \) and \( h = \sigma_1/\sigma_2 \), is exploited to obtain a Stieltjes integral representation for \( F(s) = 1 - m(h) \), where \( s = 1/(1 - h) \). The integral representation involves the spectral measure \( \mu \) of a self-adjoint operator that depends only on the composite geometry. The support of \( \mu \) lies in the interval \([0, 1]\). The mass of \( \mu \) is \( p_1 \), the volume fraction of medium 1. The analytic continuation method yields a sequence of increasingly tighter bounds that include the arithmetic and harmonic mean bounds and the Hashin–Shtrikman bounds. Information on the geometry of the medium is incorporated into the bounds through the moments of \( \mu \).

However, these bounds do not incorporate key information about the separation of inclusions, which is important in estimating the effective properties of high contrast composites. Bruno (1991) advanced the incorporation of separation information within the analytic continuation approach by introducing the class of matrix particle composites, and related the separation of the phases to gaps in the support of the spectral measure \( \mu \) at the ends of the interval \([0, 1]\).

A matrix particle composite consists of a matrix of conductivity \( \sigma_2 \) containing non-touching inclusions of conductivity \( \sigma_1 \). A particular case of such a composite is a q-material: spheres or circles of radius \( r_1 \) filled with material 1 are surrounded by a corona with outer radius \( r_2 \) filled with material 2 and \( q = r_1/r_2 < 1 \). As \( q \to 1 \), the corona vanishes, and the particles of material 1 are allowed to touch.

For a q-material in finite rectilinear regions in dimensions 2 and 3, Bruno found explicit formulas for the endpoints of the interval containing the zeros and poles of \( m(h) \), corresponding to the interval of support of the spectral measure \( \mu \). Bruno applied these results with the analytic continuation method to obtain bounds on the effective conductivity of random matrix particle composites. The bounds yield good estimates on \( \sigma^* \) even in the limiting high contrast cases of \( h = 0 \) or \( h = \infty \), and represent improvements on the classical arithmetic and harmonic mean bounds and the Hashin–Shtrikman bounds. The matrix particle bounds were subsequently extended to media with complex parameters by Sawicz & Golden (1995) and Golden (1997) and applied to estimating the effective complex permittivity of sea ice, extending earlier analysis that made use of the complex elementary and Hashin–Shtrikman bounds.

The inverse problem of recovering information about the microgeometry of a composite from measurements of its effective complex permittivity was first introduced by McPhedran et al. (1982) and McPhedran & Milton (1990) in the context of estimating the volume fractions in a two phase mixture. An analytical approach to bounding microstructural parameters, in particular volume fractions, is developed in (Cherkaeva & Tripp 1996; Tripp et al. 1998; Cherkaeva & Golden 1998) and applied to the estimation of brine volume in sea ice in (Cherkaeva & Golden 1998; Gully et al. 2007).

The problem is a particular case of inverse homogenization: recovery of structural information through identification of the spectral measure \( \mu \) from
effective property data. Uniqueness of the spectral measure is established in (Cherkaev 2001) and the theory is further developed in (Cherkaev 2003; Cherkaev & Zhang 2003; Cherkaev & Ou 2008; Bonifasi-Lista & Cherkaev 2008; Zhang & Cherkaev 2009).

Here we consider a reduced inverse spectral problem for matrix particle composites: recovery of bounds on the spectral gap, and hence bounds on \( q \). In particular, we consider \( q \)-materials whose high contrast constituents have volume fractions \( p_1 = p \) and \( p_2 = 1 - p \). Given data on the effective complex permittivity \( \varepsilon^* \), the complex matrix particle bounds constructed by Sawicz & Golden (1995) and Golden (1997) are inverted to obtain admissible regions in \((p, q)\)-parameter space, with explicitly computed algebraic curves forming the boundaries. For fixed \( p \), the bounds on \( q \) represent the first rigorous inversion for separation or connectedness information on the inclusions in a composite material.

We apply the results to obtain information about the microstructure of sea ice from its effective complex permittivity. One motivation for determining such inverse bounds comes from remote electromagnetic sensing of polar ice packs: brine inclusion separation may be used to monitor the brine percolation threshold (Golden et al. 1998; Golden et al. 2007), an on-off switch for fluid flow through sea ice that mediates a broad range of biological and climatic processes.

Although we consider sea ice as an example, the inversion algorithm we present may be generalized to other composites and other effective parameters. The simplicity and generality of the suggested method indicates wide potential applicability and advances the theory of inverse homogenization for recovering structural parameters from bulk property measurements.

Before embarking on its applications to sea ice, let us describe the general algorithm. The forward bounds of the analytic continuation method all belong to the special class of Möbius transformations. These are complex functions of the form \( T(z) = (Az + B)/(Cz + D) \) whose coefficients \( A, B, C, D \) are usually complex numbers. However, for the Möbius transformations arising in the theory, these coefficients are generally polynomial functions of certain structural parameters—such as \( p \) and \( q \)—that we are interested in estimating. The problem is to find the ‘good’ parameter values that allow the forward bounds to capture an observed effective permittivity. This problem is essentially equivalent to a search for those parameter values that allow \( \varepsilon^* = T(z) \) to be solved for some real number \( z = \hat{z} \) known as the spectral parameter. Here \( T(z) \) describes one of the forward bounding circles. The process of solving \( \varepsilon^* = T(z) \) yields an algebraic equation in the structural parameters whose solution bounds the region of ‘good’ parameter values within a larger parameter space. We present the general form of this algebraic equation. In different applications this algebraic equation will take different forms. If there are two parameters of interest the solution of this algebraic equation is a 1-dimensional curve that lends itself well to visual display.

2. Sea ice and its effective complex permittivity

Sea ice is a mixture of pure ice, brine, and air. In cold first year ice, brine is typically concentrated in sub-millimeter scale pockets. Although the local complex permittivity \( \varepsilon(x) \) varies considerably on the millimeter scale, an electromagnetic wave of sufficiently long wavelength cannot resolve the fine scale variation between
between ice, brine, and air. This is the case for the Synthetic Aperture Radar
used in remote sensing that operates in the C-band—a nominal frequency range
of 8 to 4 GHz with a corresponding wavelength range of 3.75 to 7.5 cm. For such
long wavelengths, sea ice may be treated as if it were a homogeneous material
having a single effective complex permittivity \( \varepsilon^* \). In the long wavelength regime
the wavelength is assumed to be infinite—currently a necessary assumption for
the analytic continuation method.

Here we treat sea ice as a two component medium instead of a three component
medium. The first phase consists of brine, retained as a pure medium, having
complex permittivity \( \varepsilon_1 \). The second phase is an ice-air composite having an
effective complex permittivity \( \varepsilon_2 \) that is approximated by a mixing formula
incorporating the relatively close \( \varepsilon_{\text{air}} \) and \( \varepsilon_{\text{ice}} \). Section 6 elaborates on this
mixing formula. In the sequel the second ‘ice phase’ refers to this composite of
pure ice and air. Although the three component case can also be treated with
multicomponent bounds (Golden 1986; Milton 1987a, 1987b; Milton & Golden
1990) the mathematics involves several complex variables and has a number of
unresolved issues.

The tightest of the forward bounds are obtained in §3 b (b.3) by assuming that
the sea ice is both statistically isotropic and is a matrix particle composite. In
actual sea ice the brine inclusions tend to be elongated in the vertical direction.
Because of this, we take the dimension \( d = 2 \), so that an assumption of statistical
isotropy effectively reduces to an assumption that the geometry is isotropic only
within the horizontal plane. This is consistent with the data set analyzed in
§7 which comes from measurements of ice slabs using vertically incident waves.
Except where dimension \( d \) is explicitly mentioned, all forward and inverse bounds
assume \( d = 2 \).

Although this two dimensional, two component model works well for sea ice, it
may not be viable for other composites such as the Ag-MgF\(_2\) cermet films studied
by Gajdardziska-Josifovska et al. (1989) who point out that three-phase cermets
are evidently not amenable to accurate modeling by two-phase systems.

3. The forward theory

This section summarizes the analytic continuation method (Bergman 1978; Milton
1980; Golden & Papanicolaou 1983; Cherkaev 2001; Zhang & Cherkaev 2009)
focusing in particular on the problem of obtaining forward bounds on the effective
complex permittivity of sea ice. We also summarize the work of Bruno (1991). We
obtain four types of forward bounds: the first and second order bounds \( R_1 \) and \( R_2 \),
and the first and second order matrix particle bounds \( R_{1mp} \) and \( R_{2mp} \). Each of these
incorporates different assumptions about the sea ice geometry: \( R_1 \) assumes that
the brine volume fraction is known; \( R_2 \) assumes in addition that the distribution
of the brine is statistically isotropic. The same holds for \( R_{1mp} \) and \( R_{2mp} \), with the
yet additional assumption of a matrix particle model of sea ice.

The analytic continuation method models sea ice as a two phase random
medium in all of \( \mathbb{R}^d \), with an isotropic local complex permittivity \( \varepsilon(x, \beta) \), with
\( \varepsilon(x, \beta) \) a stationary random field in \( x \in \mathbb{R}^d \) and \( \beta \in \Omega \), where \( \Omega \) is the set
of all realizations of the random medium. The complex permittivity \( \varepsilon(x, \beta) \)
takes values $\varepsilon_1$ and $\varepsilon_2$, the permittivities of brine and ice, respectively, and we write $\varepsilon(x, \beta) = \varepsilon_1 \chi_1(x, \beta) + \varepsilon_2 \chi_2(x, \beta)$, where $\chi_1$ is the characteristic function of medium 1, which equals one for all realizations $\beta \in \Omega$ having medium 1 at $x$, and equals zero otherwise, and $\chi_2 = 1 - \chi_1$.

The constitutive relation can be written as $D = \varepsilon E$, where $E(x, \beta)$ and $D(x, \beta)$ are the stationary random electric and displacement fields, satisfying equations

$$\nabla \cdot D = 0, \quad \nabla \times E = 0,$$  

(3.1)

We assume that $(E(x, \beta)) = e_j$, where $e_j$ is a unit vector in the $j^{th}$ direction, for some $j = 1, \ldots, d$, and $\langle \cdot \rangle$ means ensemble average over $\Omega$ or spatial average over all of $\mathbb{R}^d$. The effective complex permittivity tensor $\varepsilon^*$ is defined as

$$\langle D \rangle = \varepsilon^* \langle E \rangle.$$  

(3.2)

Here we are dealing with isotropic composites, so we consider only one diagonal coefficient of the effective permittivity tensor $\varepsilon^* = \varepsilon_{jj}$.

Homogeneity of the effective parameter, $\varepsilon^*(a \varepsilon_1, a \varepsilon_2) = a \varepsilon^*(\varepsilon_1, \varepsilon_2)$, applied with $a = 1/\varepsilon_2$, results in $\varepsilon^*(\varepsilon_1/\varepsilon_2, 1) = \varepsilon^*(\varepsilon_1, \varepsilon_2)/\varepsilon_2$. Hence by introducing $h = \varepsilon_1/\varepsilon_2$, we can consider the effective complex permittivity formed by constituents with the parameters $h$ and 1. We define $m(h)$ by $m(h) = \varepsilon^*(\varepsilon_1, \varepsilon_2)/\varepsilon_2$.

The function $m(h)$ is analytic off the real negative axis $(-\infty, 0)$ in the $h$-plane and maps the upper half plane to the upper half plane: this characterizes $m(h)$ as a Herglotz function (Baker & Graves-Morris 1996, p. 262). A Herglotz function has the integral representation

$$\phi(z) = a z + \beta + \int_{-\infty}^{\infty} \frac{z u + 1}{u - z} d\nu(u), \quad \beta \in \mathbb{R}, \quad a > 0,$$

with $\nu(u)$ bounded and nondecreasing on $\mathbb{R}$. If the first moment of $\nu$ is finite we may rewrite this as

$$\phi(z) = a z + \beta' + \int_{-\infty}^{\infty} \frac{d\mu(u)}{u - z}; \quad \beta' = \beta - \int_{-\infty}^{\infty} u d\nu(u), \quad d\mu(u) = (1 + u^2) d\nu(u).$$

This representation allows us to write an analytic integral representation for $\varepsilon^*$. For this purpose it is more convenient to introduce $s = 1/(1 - h)$ and consider $F(s) = 1 - m(h)$, which is analytic off $[0, 1]$ in the $s$-plane. Then

$$F(s) = 1 - \frac{\varepsilon^*}{\varepsilon_2} = \int_{0}^{1} \frac{d\mu(z)}{s - z}, \quad s = \frac{1}{1 - h},$$  

(3.3)

where $\mu$ is a positive measure on $[0, 1]$. This formula is essentially the spectral representation of the resolvent $E = (s + \Gamma_{\chi_1})^{-1} e_j$, obtained from (3.1) and (3.2), where $\Gamma = \nabla(-\Delta)^{-1} \nabla$, $\Delta$ denotes the Laplacian, and $(-\Delta)^{-1}$ is convolution with the free-space Green’s function for $-\Delta$. In the Hilbert space $L^2(\Omega, P)$ with weight $\chi_1$ in the inner product, $\Gamma_{\chi_1}$ is a bounded self adjoint operator with norm less than or equal to one. In (3.3), $\mu$ is a spectral measure of $\Gamma_{\chi_1}$. One of the most important features of (3.3) is that it separates the parameter information in $s = \varepsilon_2/(\varepsilon_2 - \varepsilon_1)$ from information about the geometry of the mixture, which is all contained in $\mu$. 


Statistical assumptions about the geometry are incorporated into $\mu$ through its moments $\mu_n$. A comparison of the perturbation expansion of (3.3) around a homogeneous medium, $s = \infty$ or equivalently $\varepsilon_1 = \varepsilon_2$, namely

$$F(s) = \mu_0 s^{-1} + \mu_1 s^{-2} + \mu_2 s^{-3} + \cdots,$$

with a similar expansion of the resolvent representation for $F(s)$ yields $\mu_n = \int_0^1 z^n d\mu(z) = (-1)^n \langle \chi_1 [(\Gamma \chi_1)^n e_j \cdot e_j \rangle$. The zeroth moment $\mu_0 = p_1$ where $p_1$ is the volume fraction of the first material in the composite, and for a statistically isotropic composite material, the first moment of $\mu$ is calculated as $\mu_1 = p_1 p_2 d^{-1}$.

Expansion (3.4) converges only in the disc $|h^{-1}| < 1$, while the integral representation (3.3) provides the analytic continuation of (3.4) to the full domain of analyticity. In this way, information obtained about a nearly homogeneous system can be used to analyze the system near percolation as $h \to 0$ or $h \to \infty$.

(a) First and second order bounds

Bounds on $\varepsilon^*$, or $F(s)$, are obtained by fixing $s$ in (3.3), varying over admissible measures $\mu$, and finding the corresponding range of values of $F(s)$ in the complex plane. Two types of bounds on $\varepsilon^*$ are readily obtained. The first order bounds $R_1$ assume only that the relative volume fractions $p_1$ and $p_2 = 1 - p_1$ are known, so that only $\mu_0 = p_1$ need be satisfied. The second order bounds $R_2$ assume in addition that the material is statistically isotropic.

(a.1) The forward region $R_1$

The set of admissible measures satisfying $\mu_0 = p_1$ forms a compact, convex set. Since (3.3) is a linear functional of $\mu$, the extreme values of $F(s)$ are attained by extremes of the admissible measures: these are the Dirac point measures of the form $p_1 \delta_z$. The values of $F(s)$ are therefore bounded by the circle

$$C_1(z) = \frac{p_1}{s - z}, \quad -\infty \leq z \leq \infty, \quad \text{(relevant arc: } 0 \leq z \leq p_2). \quad (3.5)$$

A second circle bounding $R_1$ may be obtained by introducing the function

$$E(s) = 1 - \frac{\varepsilon_1}{\varepsilon^*} = \frac{1 - sF}{s(1 - F)}.$$ 

Bergman (1982) established that this is a Herglotz function like $F(s)$, analytic off $[0, 1]$, with a representation like (3.3) whose representing measure has mass $p_2$, i.e.,

$$E(s) = \int_0^1 \frac{d\xi(z)}{s - z}, \quad \xi_0 = \int_0^1 d\xi(z) = p_2. \quad (3.6)$$

Then in the $E$-plane, the other circular boundary of $R_1$ is parameterized by

$$\tilde{C}_1(z) = \frac{p_2}{s - z}, \quad -\infty \leq z \leq \infty, \quad \text{(relevant arc: } 0 \leq z \leq p_1). \quad (3.7)$$

After these circles are transferred to the common $\varepsilon^*$-plane, and noting their intersection, the relevant bounding arcs given parenthetically in (3.5) and (3.7) may be determined.
(a.2) The forward region $R_2$

If the material is further assumed to be statistically isotropic, i.e., $\varepsilon_{ik}^* = \varepsilon^* \delta_{ik}$, then $\mu_1 = p_1 p_2 d^{-1}$ must be satisfied as well, and we obtain the second order bounds $R_2$. Now instead of directly varying over all those admissible measures whose moments satisfy both $\mu_0 = p_1$ and $\mu_1 = p_1 p_2 d^{-1}$, it is convenient to use the following transformation, as pointed out by Bergman (1982):

$$F_1(s) = \frac{1}{p_1} - \frac{1}{s F(s)}.$$  \hspace{1cm} (3.8)

The function $F_1(s)$ is also an Herglotz function, and has the representation

$$F_1(s) = \int_0^1 \frac{d\mu^1(z)}{s - z}.$$  \hspace{1cm} (3.9)

The constraint (3.9) on $F(s)$ is then transformed to a restriction of only the mass of $\mu^1$, which is $\mu^1_0 = p_2 (p_1 d)^{-1}$. Applying the same procedure that was used for $R_1$ yields the region $R_2$, whose boundaries are again circular arcs. One arc, in the $F$-plane, is

$$C_2(z) = \frac{p_1(s-z)}{s(s-z - p_2/d)}, \hspace{1cm} 0 \leq z \leq (d-1)/d.$$  \hspace{1cm} (3.10)

In the $E$-plane, the other arc is

$$\tilde{C}_2(z) = \frac{p_2(s-z)}{s(s-z - p_1 (d-1)/d)}, \hspace{1cm} 0 \leq z \leq 1/d.$$  \hspace{1cm} (3.11)

The forward bounds discussed up to this point are summarized in table 1: on the left hand side are the bounds on the values $F(s)$ and $E(s)$, which arise from the integral representations of the form (3.3) and (3.6) by letting the representing measure vary over the extremes. In order to be useful as bounds on the complex permittivity, these should be transferred to the $\varepsilon^*$-plane using the relations

$$F(s) = 1 - \frac{\varepsilon^*}{\varepsilon_2}, \hspace{1cm} E(s) = 1 - \frac{\varepsilon_1}{\varepsilon^*}.$$  \hspace{1cm} (3.12)

The entries in the right hand side of table 1 are obtained by transferring such bounds accordingly. Some notational simplification is achieved by introducing the new variable $\theta = 2s - 1$. Note that each $T_{i,j}(z; p)$, $i, j = 1, 2$, is a Möbius transformation that maps the extended real line onto a circle in the $\varepsilon^*$-plane.

(a.3) Isomorphic groups

A convenient way of transferring bounds between planes exploits the isomorphism between the Möbius transformation group and the projective general linear group $PGL(2, \mathbb{C})$ (Jones & Singerman 1987). For example, the relationship between $\varepsilon^*$ and $F$ given by (3.12) has the matrix representations, with $s$ fixed,

$$T_{F \rightarrow \varepsilon^*} \overset{\sim}{=} \begin{pmatrix} -\varepsilon_2 & \varepsilon_2 \\ 0 & 1 \end{pmatrix}, \hspace{1cm} T_{\varepsilon^* \rightarrow F} \overset{\sim}{=} \begin{pmatrix} -1 & \varepsilon_2 \\ 0 & \varepsilon_2 \end{pmatrix}.$$
The very bounds derived by Hashin & Shtrikman (1962).

Table 1. Forward bounds on $\varepsilon^*$: forward bounds on $E(s)$ and $F(s)$ are on the left. The result of translating these bounds to the $\varepsilon^*$-plane are on the right. In making the translation we assume $d = 2$. Notation: $s = \varepsilon_2/(\varepsilon_2 - \varepsilon_1)$, $\theta = 2s - 1$, $p = p_1 = 1 - p_2$.

<table>
<thead>
<tr>
<th>$\mathcal{R}_1$, first arc:</th>
<th>$\mathcal{R}_1$, second arc:</th>
<th>$\mathcal{R}_2$, first arc:</th>
<th>$\mathcal{R}_2$, second arc:</th>
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<tr>
<td>$C_1(z) = \frac{p_1}{s - z}$</td>
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<td>$C_2(z) = \frac{p_1(s - z)}{s(s - z - p_1/d)}$</td>
<td>$\tilde{C}_2(z) = \frac{p_2(s - z)}{s(s - z - p_1(d - 1)/d)}$</td>
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<tr>
<td>$T_{1,1}(z; p) = \frac{-\varepsilon_2 z - \varepsilon_2 p + \varepsilon_2 s}{-z + s}$</td>
<td>$T_{1,2}(z; p) = \frac{-\varepsilon_2 + \varepsilon_1 s}{-z + p + s - 1}$</td>
<td>$T_{2,1}(z; p) = \frac{-2\varepsilon_2(\theta + 1 - 2p)z + \varepsilon_2(\theta + 1)(\theta - p)}{-2(\theta + 1)z + (\theta + 1)(\theta + p)}$</td>
<td>$T_{2,2}(z; p) = \frac{-2\varepsilon_2(\theta - 1)z + \varepsilon_2(\theta - 1)(\theta + 1 - p)}{-2(\theta - 1 + 2p)z + (\theta + 1)(\theta + p)}$</td>
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Then with $p = p_1$, multiplying a matrix (in the equivalence class) representing $C_1(z)$ on the left by $T_{\{E\rightarrow\varepsilon^*\}}$ yields a matrix representation for $T_{1,1}(z; p)$:

$$
\begin{pmatrix}
-\varepsilon_2 & \varepsilon_2 \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
0 & p \\
-1 & s
\end{pmatrix}
= \begin{pmatrix}
-\varepsilon_2 & -\varepsilon_2 p + \varepsilon_2 s \\
-1 & s
\end{pmatrix}.
$$

The other entries on the right hand side of Table 1 may be obtained similarly. Let us note that $T_{\{E\rightarrow\varepsilon^*\}} = (0 \; \varepsilon_1; -1 \; 1)$ and $T_{\{E\rightarrow F\}} = (-s \; 1; -s \; s)$.

(a.4) The classical bounds

In the $\varepsilon^*$-plane the two arcs describing $\mathcal{R}_1$ meet at the vertices

$$
T_{1,1}(z; p)\big|_{z = p_2} = T_{1,2}(z; p)\big|_{z = 0} = (p_1/\varepsilon_1 + p_2/\varepsilon_2)^{-1},
$$

$$
T_{1,1}(z; p)\big|_{z = 0} = T_{1,2}(z; p)\big|_{z = p_1} = p_1 \varepsilon_1 + p_2 \varepsilon_2.
$$

When $\varepsilon_1$ and $\varepsilon_2$ are real, $\mathcal{R}_1$ reduces to the interval defined by the classical harmonic mean and arithmetic mean bounds: $(p_1/\varepsilon_1 + p_2/\varepsilon_2)^{-1} \leq \varepsilon^* \leq p_1 \varepsilon_1 + p_2 \varepsilon_2$. Similarly when $\varepsilon_1$ and $\varepsilon_2$ are real with $\varepsilon_1 \geq \varepsilon_2$, $\mathcal{R}_2$ collapses to the interval

$$
\varepsilon_2 + p_1 \left( \frac{1}{\varepsilon_1 - \varepsilon_2} + \frac{p_2}{d \varepsilon_2} \right)^{-1} \leq \varepsilon^* \leq \varepsilon_2 + p_2 \left( \frac{1}{\varepsilon_2 - \varepsilon_1} + \frac{p_1}{d \varepsilon_1} \right)^{-1},
$$

the very bounds derived by Hashin & Shtrikman (1962).
(b) First and second order matrix particle bounds

Still tighter bounds on $\varepsilon^*$, $\mathcal{R}^{mp}_1 \subseteq \mathcal{R}_1$ and $\mathcal{R}^{mp}_2 \subseteq \mathcal{R}_2$, may be obtained if the material has a matrix particle structure with separated inclusions. In this case, the support of the spectral measure $\mu$ in (3.3) is contained in the subinterval $[s_m, s_M]$ and

$$F(s) = 1 - \frac{\varepsilon^*}{\varepsilon_2} = \int_{s_m}^{s_M} \frac{d\mu(z)}{s - z}. \quad (3.13)$$

This important observation is due to Bruno (1991), whose work we summarize next. Although Bruno considers the effective conductivity of strongly heterogeneous composites, the mathematics of effective complex permittivity is identical.

(b.1) Summary of Bruno’s work

The bounds $s_m$ and $s_M$ are obtained by mapping the bounds on the singularities and zeros of the corresponding function $m(h)$ from the complex $h$-plane to the $s$-plane. The $h$-plane bounds result from analyticity of $m(h)$, corresponding to a matrix particle composite, in neighborhoods of $h = 0$ and $h = \infty$. The method is based on an expansion of the electric potential $\phi$ into convergent series: in $h$ around $h = 0$; in $w = 1/h$ around $h = \infty$.

To sketch the argument, we consider a domain $\mathcal{D}$ large in comparison with the size of inhomogeneity, $\mathcal{D} = \{0 \leq x_i \leq 1\}$, filled with composite mixture of two materials with properties $\varepsilon_1 = h$ and $\varepsilon_2 = 1$. We assume that an electric potential $\phi$ is constant on the upper $\partial_1$ and lower $\partial_0$ boundaries and periodic on vertical boundaries $S$ of the domain $\mathcal{D}$, so that $\phi$ satisfies the equation:

$$\nabla \cdot \varepsilon(x) \nabla \phi(x) = 0 \quad \text{in} \; \mathcal{D}, \quad \phi(x)|_{\partial_0} = 0, \quad \phi(x)|_{\partial_1} = 1, \quad \frac{\partial \phi(x)}{\partial n}|_S = 0. \quad (3.14)$$

Using the solution of (3.14), the effective conductivity $m(h)$ may be calculated as:

$$m(h) = \int_{\mathcal{D}} \varepsilon(x)|\nabla \phi(x)|^2 \, dx = h \int_{\mathcal{D}_\chi} |\nabla \phi(x)|^2 \, dx + \int_{\mathcal{D}'} |\nabla \phi(x)|^2 \, dx, \quad (3.15)$$

where $\mathcal{D}_\chi \subseteq \mathcal{D}$ is the part of $\mathcal{D}$ occupied by the material with conductivity $h$, and $\mathcal{D}' = \mathcal{D} - \mathcal{D}_\chi$. It is known that (3.14) has a unique solution for any value of $h$ outside the negative real axis (Bergman 1978; Golden & Papanicolaou 1983) and that $m(h)$ as an analytic function of $h \in \mathbb{C}/(-\infty, 0]$.

Using a combination of the trace and extension theorems (Nečas 1967) and the Poincare inequality for functions in $H^1(\mathcal{D}_\chi)$ and $H^1(\mathcal{D}')$, it can be shown that for the matrix particle composites, the two integrals in the right hand side of (3.15) are bounded: each function $u' \in H^1(\mathcal{D}')$ can be extended to a function $u \in H^1(\mathcal{D})$ which coincides with $u'$ in $\mathcal{D}'$ and

$$\int_{\mathcal{D}_\chi} |\nabla u(x)|^2 \, dx \leq A \int_{\mathcal{D}'} |\nabla u'(x)|^2 \, dx; \quad (3.16)$$
and for each function \( u \in H^1(D_x) \) there is a function \( u' \in H^1(D') \) which differs by a constant from \( u \) on the boundary of each inclusion, and
\[
\int_{D'} |\nabla u'(x)|^2 \, dx \leq B \int_{D_x} |\nabla u(x)|^2 \, dx.
\]
(3.17)
The fields in matrix particle composites with corona around grain inclusions satisfy these bounds with positive constants \( A \) and \( B \) depending on grain shape and separation.

To show analyticity of \( m(h) \) around the origin, the solution of (3.14) is represented as
\[
\phi(x, h) = \sum_{k=0}^{\infty} \phi_k(x) h^k,
\]
(3.18)
with the coefficients \( \phi_k \) satisfying an infinite system of equations obtained from (3.14) upon substitution of the series (3.18). Separating the problem into two problems over subdomains \( D_x \) and \( D' \) allows one to solve them iteratively, since the problems are coupled through the condition on the boundary of inclusions. Using (3.16), one can show that (3.18) as well as the series of the gradients \( \nabla \phi_k \) is absolutely convergent for \( |h| \leq 1/A \). Therefore \( \phi(x, h) \) and hence \( m(h) \) is analytic for \( |h| \leq 1/A \). Similarly, to show analyticity of \( m(h) \) at infinity, \( \phi(x, h) = \psi(x, w = h^{-1}) \) is expanded as
\[
\psi(x, w) = \sum_{k=0}^{\infty} \psi_k(x) w^k,
\]
(3.19)
around the origin in the \( w \)-plane. Using (3.17) the convergence of (3.19) can be shown for \( |w| \leq 1/B \).

Together (3.18) and (3.19) provide the analytic continuation of \( \phi(x, h) \) in the regions \( |h| \leq 1/A \) and \( |h| \geq B \). Accordingly, \( m(h) \) is analytic in these regions, and in particular, for \( h \) on the negative real axis, \( -1/A \geq h \) and \( h \leq -B \). Mapping the interval \([-B, -1/A]\) to the \( s \)-plane gives the subinterval \( s_m \leq \zeta \leq s_M \) bounding the support of the measure \( \mu \) displayed in (3.13), with \( s_m \) and \( s_M \) depending on the microgeometry of the composite.

The further the separation of the inclusions, the smaller the support interval \([s_m, s_M]\), and the tighter the bounds. Explicit calculations for \( s_m \) and \( s_M \) are available for the following matrix particle model of sea ice: within the horizontal plane, the brine is assumed to be contained in separated, circular discs of radii \( r_{\text{brine}} \), holding random positions in such a way that each disc of brine is surrounded by a corona of ice, with outer radius \( r_{\text{ice}} \). As introduced in §1, this is a \( q \)-material with \( q = r_{\text{brine}}/r_{\text{ice}} \). For such a geometry, Bruno has calculated for \( d = 2 \),
\[
s_m = \frac{1}{2}(1 - q^2), \quad s_M = \frac{1}{2}(1 + q^2).
\]
(3.20)
Smaller \( q \) values indicate well separated brine—and colder temperatures as figure 5 indicates—and \( q = 1 \) corresponds to no restriction on the separation, with \( s_m = 0 \) and \( s_M = 1 \), so that \( \mathcal{R}_{1}^{mp} \) and \( \mathcal{R}_{2}^{mp} \) coincide with \( \mathcal{R}_1 \) and \( \mathcal{R}_2 \).
Returning to (3.13), a convenient way of incorporating the support restriction is the substitution

$$ s = \lambda t + s_m, \quad \lambda = s_M - s_m = q^2, $$

(3.21)

which maps $[s_m, s_M]$ in the $s$-plane to $[0, 1]$ in the $t$-plane. Consequently

$$ H(t) = F(s) = F(\lambda t + s_m) $$

(3.22)

is analytic off $[0, 1]$ in the complex $t$-plane and there is a positive Borel measure $\nu$ on $[0, 1]$ such that $H(t) = \int_0^1 (t - z)^{-1} d\nu(z)$. Using $\mu_0 = p_1$, $\mu_1 = p_1 p_2 d^{-1}$ it can be shown that $\nu$ has moments

$$ \nu_0 = \frac{p_1}{\lambda}, $$

(3.23a)

$$ \nu_1 = \frac{p_1}{\lambda^2} \left( \frac{p_2}{d} - s_m \right), $$

(3.23b)

with the formula for $\nu_1$ holding under the assumption of statistical isotropy.

(b.2) The forward region $R_{1_{mp}}^m$

The bounds $R_{1_{mp}}^m$ are obtained by assuming (3.23a) is satisfied. Applying the same extremal procedure that gave (3.5) for $R_1$ shows that the values of $H(t)$ lie inside the circle

$$ K_1(z) = \frac{p_1/\lambda}{t - z}, \quad z \in \mathbb{R}. $$

Note that $H(t)$ assumes values in the $F$-plane: the $H$- and $F$-planes coincide. This translates via (3.21) and (3.22) into the circle $K_1'(z) = p_1/(s - \lambda z - s_m), \quad z \in \mathbb{R}$, which is readily seen to coincide with the image of $C_1(z)$. So in this case the matrix particle assumption provides no improvement over the first arc of $R_1$.

Next we consider the analog $G(t)$ of $E(s)$ defined by

$$ G(t) = \frac{1 - tH(t)}{t(1 - H(t))}. $$

(3.24)

Then $G(t)$ has an integral representation $G(t) = \int_0^1 (t - z)^{-1} d\rho(z)$, where the mass of $\rho$ is $\rho_0 = 1 - \lambda^{-1} p_1$. We then obtain a circle in the $G$-plane analogous to $\hat{C}_1(z)$ in (3.7), namely,

$$ \hat{K}_1(z) = \frac{1 - \lambda^{-1} p_1}{t - z}, \quad z \in \mathbb{R}. $$

(3.25)

In the $F$-plane this becomes, via (3.22) and (3.24),

$$ \hat{K}_1'(z) = \frac{p_1(s - s_m) - \lambda^2 z}{(s - s_m)(p_1 - \lambda + s - s_m) - \lambda(s - s_m) z}, \quad z \in \mathbb{R}, $$

(3.26)

which improves upon (3.7). Here (3.26) is a correction of (Golden 1997, (3.29)).
The allowed values of \( q \) make the translation we assume and representation in terms of a measure \( q \), if

\[
R = \frac{1}{2}, \quad \text{second arc: } mp
\]

The other circle is obtained by applying a similar transformation to \( G(t) \):

\[
G_1(t) = \frac{1}{\rho_0} - \frac{1}{tG(t)} = \frac{\lambda}{\lambda - p_1} - \frac{1}{tG(t)}.
\]
This function is also Herglotz, analytic off \([0, 1]\), with representing measure \(\rho^1\). The mass of \(\rho^1\) is

\[
\rho_0^1 = \frac{\nu_0(1 - \nu_0) - \nu_1}{(1 - \nu_0)^2}.
\] (3.31)

The allowed values of \(G_1(t)\) are contained inside the circle \(\{\rho_0^1/(t - z) : z \in \mathbb{R}\}\), which in the \(G\)-plane becomes:

\[
\hat{K}_2(z) = \frac{(1 - \nu_0)(t - z)}{t(t - z - \nu_0 + \nu_1/(1 - \nu_0))}, \quad z \in \mathbb{R}.
\] (3.32)

Table 2 summarizes the first and second order matrix particle bounds: the left hand side gives bounds on the values of \(G(t)\) and \(H(t)\), which are then transferred to the \(\varepsilon^*\)-plane on the right hand side. For example, the matrix representation of \(T_{2,2}(z;p,q)\) may be obtained by multiplying the matrix representing \(\hat{K}_2(z)\) on the left by \(T_{\{G \rightarrow \varepsilon^*\}} = T_{\{F \rightarrow \varepsilon^*\}}T_{\{G \rightarrow F\}}\), i.e.,

\[
\begin{pmatrix}
-\varepsilon_2 & \varepsilon_2 \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
-1 & t^{-1} \\
-1 & 1
\end{pmatrix}
\begin{pmatrix}
-1 + \nu_0 & t(1 - \nu_0) \\
-\nu_0 & t(t - \nu_0 + \nu_1(1 - \nu_0)^{-1})
\end{pmatrix}
\]

\[
= \begin{pmatrix}
\varepsilon_2 t^{-1} - \varepsilon_2 & (\varepsilon_2 t^{-1} - \varepsilon_2) t(1 - \nu_0 + \nu_1(1 - \nu_0)^{-1}) \\
1 - \nu_0 - t & -t(1 - \nu_0) + t(t - \nu_0 + \nu_1(1 - \nu_0)^{-1})
\end{pmatrix}
\]

and then substituting \(t = (\theta + q^2)/(2q^2)\), \(\nu_0 = p/q^2\), and \(\nu_1 = p(q^2 - p)/(2q^4)\) from (3.20), (3.21), and (3.23). Typical forward bounds on \(\varepsilon^*\) are illustrated in figures 1 and 3. Figure 3 shows \(\mathcal{R}_1\) (outer dashed), \(\mathcal{R}_2\) (inner dashed), \(\mathcal{R}_1^{mp}\) (outer solid), \(\mathcal{R}_2^{mp}\) (inner solid).

4. The inverse problem

Having computed the forward bounds we now formulate the general inverse problem: given an observed effective property, determine the range of parameter values consistent with the observation. This is illustrated in figure 1 using sea ice modeled as a two component random media, effective complex permittivity \(\varepsilon^*\) as the observed effective property, and brine volume fraction \(p\) as the parameter of interest. As the brine volume increases from \(p \approx .007\) to \(p \approx .040\), the forward region \(\mathcal{R}_1\) changes size and sweeps over the fixed observed \(\varepsilon^*\), while the smaller region \(\mathcal{R}_2\) covers \(\varepsilon^*\) only for \(p\) between \(p \approx .012\) and \(p \approx .024\). These two intervals, respectively, are the first and second order inverse bounds on \(p\), given the observed \(\varepsilon^*\). It turns out that the end points of these intervals may be determined as roots of the polynomials \(F_{i,j}(p)\) defined in §5 by inverting \(T_{i,j}(z;p)\), \(i, j = 1, 2\).

Simultaneous inversion for both \(p\) and \(q\) is more complicated, but the same method applies: given an observed \(\varepsilon^*\), inversion of \(T_{i,j}(z;p,q)\) determines the algebraic curve \(G_{i,j}(p, q) = 0\) that bounds a region in \((p, q)\)-parameter space.
5. The inverse algorithm

Theorem 1 provides the theoretical basis of the inverse algorithm. It asserts that the boundary of the inverse region may be computed by solving an algebraic equation involving the structural parameters. This extends and provides an alternative to the approach of Cherkaeva & Golden (1998) in which bounds for \( p \) were found by solving coupled nonlinear equations.

Theorem 1 is based on the observation that the bounds on \( \varepsilon^* \) on the right hand sides of tables 1 and 2 are all Möbius transformations in \( z \); the relevant arcs shown in figure 1 are the images of certain subintervals of \([0,1]\) under such transformations. The full circle is the image of the extended real line \( \mathbb{R} \cup \{\infty\} \). For generality we now designate structural parameters by \( \pi_1, \ldots, \pi_n \) instead of just \( p \) and \( q \). If parameter values \( \hat{\pi} = (\hat{\pi}_1, \ldots, \hat{\pi}_n) \) are chosen so that \( \varepsilon^* \) (or another observed effective property) lies on such a circle, the spectral parameter \( \hat{z} \) is defined to be the \( \hat{z} \in \mathbb{R} \) such that \( \varepsilon^* = T_{\hat{\pi}}(\hat{z}) \).

We use the following notation: \( \mathbb{C}[x_1, \ldots, x_n] \) denotes the ring of multivariate polynomials in \( x_1, \ldots, x_n \) with complex coefficients; \( \overline{z} \) is the complex conjugate of \( z \in \mathbb{C} \); both \( T_\pi(z) \) and \( T(z; \pi) \) are used to indicate the parametric dependence of a Möbius transformation on \( \pi = (\pi_1, \ldots, \pi_n) \). We use the following facts: Möbius transformations map circles to circles in \( \mathbb{C} \), where lines are regarded as circles of infinite radii; and the compositional inverse of \( T(z) = (Az + B)/(Cz + D) \) is \( T^{-1}(z) = (Dz - B)/(-Cz + A) \), see e.g. (Jones & Singerman 1987).

**Theorem 1.** Let \( T(z; \pi) \) be an \( n \)-parameter family of Möbius transformations

\[
T_\pi(z) = T(z; \pi) = \frac{A(\pi)z + B(\pi)}{C(\pi)z + D(\pi)}, \quad \pi = (\pi_1, \ldots, \pi_n)
\]

where \( A(\pi), B(\pi), C(\pi), D(\pi) \in \mathbb{C}[\pi_1, \ldots, \pi_n] \) and the parameters \( \pi_1, \ldots, \pi_n \) are real. Then a fixed \( \zeta \in \mathbb{C} \) lies on \( T(\mathbb{R}; \hat{\pi}) \), a circle with a single point removed, if
and only if \( \hat{\pi} \) is a real root of the multivariate polynomial \( F_\zeta(\pi) \) defined by

\[
F_\zeta(\pi) = \Im\{[D(\pi)\zeta - B(\pi)][-C(\pi)\zeta + A(\pi)]\},
\]

and \( \hat{\pi} \) is not also a root of the multivariate polynomial

\[
S_\zeta(\pi) = -C(\pi)\zeta + A(\pi).
\]

For such \( \hat{\pi} \), \( \zeta = T(\hat{z}; \hat{\pi}) \) where the spectral parameter \( \hat{z} \) may be computed from \( \hat{\pi} \) by

\[
\hat{z} = \frac{D(\hat{\pi})\zeta - B(\hat{\pi})}{-C(\hat{\pi})\zeta + A(\hat{\pi})} = \frac{\Re\{D(\hat{\pi})\zeta - B(\hat{\pi})\}}{\Im\{-C(\hat{\pi})\zeta + A(\hat{\pi})\}} = \frac{\Im\{D(\hat{\pi})\zeta - B(\hat{\pi})\}}{\Im\{-C(\hat{\pi})\zeta + A(\hat{\pi})\}}.
\]

**Proof.** Let \( \zeta \in \mathbb{C} \) be fixed and assume \( \zeta \in T(\mathbb{R}; \hat{\pi}) \) with \( \hat{\pi} = (\hat{\pi}_1, \ldots, \hat{\pi}_n) \). Then

\[
\zeta = T(\hat{z}; \hat{\pi}) = A(\hat{\pi})\hat{z} + B(\hat{\pi})
\]

for some \( \hat{z} \in \mathbb{R}, \hat{z} \neq \infty \). Since \( S_\zeta(\pi) = 0 \) can only occur if \( \hat{z} = \infty \) it follows that \( S_\zeta(\pi) \neq 0 \). Solving for \( \hat{z} \) by inverting (5.4) gives

\[
\hat{z} = T^{-1}(\zeta; \hat{\pi}) = \frac{D(\hat{\pi})\zeta - B(\hat{\pi})}{-C(\hat{\pi})\zeta + A(\hat{\pi})}.
\]

By considering separately the real and imaginary parts of (5.5) and using the fact that \( \hat{z} \in \mathbb{R} \), it follows that \( \pi = \hat{\pi} \) is a solution of

\[
\Im\left\{ \frac{D(\pi)\zeta - B(\pi)}{-C(\pi)\zeta + A(\pi)} \right\} = 0, \quad (\zeta \text{ fixed}).
\]

In view of \( S_\zeta(\hat{\pi}) \neq 0 \), this is equivalent to \( \hat{\pi} \) being a root of the polynomial (5.1).

In the other direction, let \( \zeta \in \mathbb{C} \) be fixed and suppose \( F_\zeta(\hat{\pi}) = 0 \) and \( S_\zeta(\hat{\pi}) \neq 0 \). Then (5.6) holds with \( \pi = \hat{\pi} \). Let \( \hat{z} \) be defined by (5.5). Then \( \zeta = T(\hat{z}; \hat{\pi}) \). Since (5.6) holds with \( \pi = \hat{\pi} \) it follows that \( \hat{z} \) is real, so (5.5) defines \( \hat{z} \) as the spectral parameter. The remaining part of (5.3) holds because for any \( z, w \in \mathbb{C}/\{0\} \), we have \( \Im\{\pi\} = 0 \) if and only if the points \( \{0, z, w\} \) are collinear, in which case \( z/w = \Re(z)/\Re(w) = \Im(z)/\Im(w) \).

Using this unified approach, we first apply theorem 1 to obtain formulas for first and second order inverse bounds on the volume fraction \( \rho \) of brine in sea-ice, and in passing rederive results of Cherkaeva & Golden (1998). Next, we apply theorem 1 to obtain first and second order inverse bounds in \((\rho, q)\)-parameter space. Since the role of \( \zeta \) will always be assumed by \( \epsilon^* \), to simplify notation we will write \( F(\rho) \) for \( F_{\epsilon^*}(\rho) \) and \( G(\rho, q) \) for \( F_{\epsilon^*}(\rho, q) \).

(a) Inverting \( \mathcal{R}_1 \)

The forward region \( \mathcal{R}_1 \) is derived assuming only knowledge of the volume fraction \( \rho = \rho_1 \). We invert \( \mathcal{R}_1 \) to obtain bounds on \( \rho \) by considering \( T_{1,1}(z; \rho) \) and \( T_{1,2}(z; \rho) \) as families of maps parameterized by \( \rho \).
(a.1) Inverting the first arc of $\mathcal{R}_1$

The polynomial coefficients of $T_{1,1}(z; p)$ are

\[ A(p) = -\varepsilon_2, \quad B(p) = -\varepsilon_2 p + \varepsilon_2 s, \quad C(p) = -1, \quad D(p) = s. \]

An application of theorem 1 gives $F_{1,1}(p) = \Im\{[\varepsilon_2 p + (\varepsilon^* - \varepsilon_2) s] [\varepsilon^* - \varepsilon_2]\}$. Solving $F_{1,1}(p) = 0$ gives a lower bound on the volume fraction:

\[ \hat{p}_{1,\ell} = \frac{[\varepsilon^* - \varepsilon_2]^2 \Im(\varepsilon_1\varepsilon_2)}{[\varepsilon_1 - \varepsilon_2]^2 \Im(\varepsilon^*\varepsilon_2)}. \] (5.7)

Note that the subscript 1 on $\hat{p}_{1,\ell}$ refers to its role as a first order bound, while $p_1$ denotes a volume fraction.

(a.2) Inverting the second arc of $\mathcal{R}_1$

The polynomial coefficients of $T_{1,2}(z; p)$ are

\[ A(p) = -\varepsilon_1, \quad B(p) = \varepsilon_1 s, \quad C(p) = -1, \quad D(p) = -1 + p + s. \]

Theorem 1 gives $F_{1,2}(p) = \Im\{[\varepsilon^* p + (\varepsilon^* - \varepsilon_1) s - \varepsilon^*] [\varepsilon^* - \varepsilon_1]\}$, and solving $F_{1,2}(p) = 0$ gives an upper bound on the volume fraction:

\[ \hat{p}_{1,u} = 1 - \frac{|\varepsilon^* - \varepsilon_1|^2 \Im(\varepsilon_2\varepsilon_1)}{|\varepsilon_2 - \varepsilon_1|^2 \Im(\varepsilon^*\varepsilon_1)}. \] (5.8)

The fact that (5.7) gives a lower bound while (5.8) gives an upper bound was determined numerically, i.e., it is the particular values of $\varepsilon_1, \varepsilon_2, \varepsilon^*$ that imply $\hat{p}_{1,\ell} \leq \hat{p}_{1,u}$.

(b) Inverting $\mathcal{R}_2$

The forward region $\mathcal{R}_2$ is the region in the $\varepsilon^*$-plane bounded by the two circles described by $T_{2,1}(z; p)$ and $T_{2,2}(z; p)$. Following the same procedure for $\mathcal{R}_2$ as $\mathcal{R}_1$, we find that each circle determines a polynomial that is quadratic in $p$, yielding the second order bounds $\hat{p}_{2,\ell}$ and $\hat{p}_{2,u}$ with $\hat{p}_{1,\ell} \leq \hat{p}_{2,\ell} \leq p \leq \hat{p}_{2,u} \leq \hat{p}_{1,u}$.

(b.1) Inverting the first arc of $\mathcal{R}_2$

Inverting $T_{2,1}(z; p)$ gives $F_{2,1}(p) = a_1 p^2 + b_1 p + c_1$ with

\[ a_1 = 23 \{ (\varepsilon^* + \varepsilon_2) \varepsilon_1 (\theta + 1) \}, \]
\[ b_1 = -2|\theta + 1|^2 \Im \{ \varepsilon^*\varepsilon_2 \} + 23 \{ (\varepsilon^* - \varepsilon_2) \varepsilon_1 \varepsilon_1 (\theta + 1) \}, \]
\[ c_1 = |\theta + 1|^2 |\varepsilon^* - \varepsilon_2|^2 \Im \{ \theta \}. \]

Solving $F_{2,1}(p) = 0$ gives the second order upper bound

\[ \hat{p}_{2,u} = \frac{-b_1 + \sqrt{b_1^2 - 4a_1c_1}}{2a_1}. \] (5.9)
(b.2) Inverting the second arc of $R_2$

Inverting $T_{2,2}(z, p)$ gives $F_{2,2}(p) = a_2 p^2 + b_2 p + c_2$ with

\[
\begin{align*}
a_2 &= 2 \Im \left\{ \epsilon^*(\theta + 1) + \epsilon_2(\theta - 1) \right\}, \\
b_2 &= 2 \Im \left\{ (\epsilon^* - \epsilon_2)(\theta^2 - 1) \right\} + \Im \left\{ [\epsilon^*(\theta + 1) + \epsilon_2(\theta - 1)](\epsilon^* - \epsilon_2)(\theta - 1) \right\}, \\
c_2 &= |\theta - 1|^2 |\epsilon^* - \epsilon_2|^2 \Im \{\epsilon\}. 
\end{align*}
\]

Solving $F_{2,2}(p) = 0$ determines the second order lower bound

\[
\hat{p}_{2,\ell} = \frac{-b_2 - \sqrt{b_2^2 - 4a_2c_2}}{2a_2}. 
\]

(5.10)

The fact that (5.9) provides an upper bound while (5.10) provides a lower bound was determined numerically, as was the determination of the sign of the radical in these equations.

(c) Inverting $R_{1}^{mp}$

The forward region $R_{1}^{mp}$ in the $\epsilon^*$-plane is determined by the two intersecting circles: $T_{1,1}(z; p, q), T_{1,2}(z; p, q), z \in \mathbb{R}$.

(c.1) Inverting the first arc of $R_{1}^{mp}$

Inversion of $T_{1,1}(z; p, q)$ reduces to (5.7) because the circular image of $K_1'(z)$ coincides with the image of $C_1(z)$, as noted in §3b (b.2).

(c.2) Inverting the second arc of $R_{1}^{mp}$

Inverting $T_{1,2}(z; p, q)$ gives the polynomial

\[
G_{1,2}(p, q) = \Im \{ [2\epsilon^*(\theta + q^2)p + (\epsilon^* - \epsilon_2)(\theta^2 - q^4)](\epsilon^*(\theta + q^2) - \epsilon_2(\theta - q^2)) \} \]

which is cubic in $q^2$. The algebraic curve $G_{1,2}(p, q) = 0$ is readily expressed as

\[
p = \frac{\Im \left\{ [(\epsilon^* - \epsilon_2)(\theta^2 - q^4)](\epsilon^*(\theta + q^2) - \epsilon_2(\theta - q^2)) \right\}}{2 \Im \{ \epsilon^*(\theta + q^2) - \epsilon_2(\theta - q^2) \}}. 
\]

(d) Inverting $R_{2}^{mp}$

The forward region $R_{2}^{mp}$ in the $\epsilon^*$-plane is described by the intersection of the two circles: $T_{2,1}(z; p, q), T_{2,2}(z; p, q), z \in \mathbb{R}$. 

\[
(5.10) 
\]
(d.1) Inverting the first arc of $R_{2}^{mp}$

Inverting $T_{2,1}(z; p, q)$ gives $G_{2,1}(p, q) = a_1(q)p^2 + b_1(q)p + c_1(q)$ with

$$a_1(q) = 2\Im \{ (\varepsilon^* + \varepsilon_2)(\theta + q^2) \},$$
$$b_1(q) = -2|\theta + q^2|^2 \Im \{ \varepsilon^* \varepsilon_2 \} + 2\Im \{ (\varepsilon^* - \varepsilon_2)\varepsilon_2\varepsilon_2\theta + q^2 \},$$
$$c_1(q) = |\theta + q^2|^2 |\varepsilon^* - \varepsilon_2|^2 \Im \{ \theta \}.$$

Note that $G_{2,1}(p, q)|_{q=1} = F_{2,1}(p)$. The algebraic curve $G_{2,1}(p, q) = 0$ is given by

$$p = \frac{-b_1(q) \pm \sqrt{|b_1(q)|^2 - 4a_1(q)c_1(q)}}{2a_1(q)}. \quad (5.11)$$

The curve $G_{2,1}(p, q) = 0$ is illustrated in figure 2; the top and bottom portions of the curve correspond to the positive and negative roots in (5.11) respectively.

Figure 2. Inverting the forward regions gives algebraic curves of this general shape; exact shape depends on $\varepsilon^*$, $\varepsilon_1$, and $\varepsilon_2$. The horizontal lines in ascending order, $p_{1,t} < p_{2,t} < p_{2,u} < p_{1,u}$, are obtained by inverting $R_1$ and $R_2$. The curves are: (a) $G_{2,2}(p, q) = 0$ from the second arc of $R_{1}^{mp}$; (b) $G_{2,1}(p, q) = 0$ from the first arc of $R_{2}^{mp}$; (c) $G_{2,1}(p, q) = 0$ from the second arc of $R_{2}^{mp}$. The larger view on the right shows (c) $G_{2,2}(p, q) = 0$; on the left this curve is not readily distinguishable from the line $p_{1,t}$.

Alternatively, and this will be used in §7,

$$G_{2,1}(p, q) = d_1(p)q^4 + e_1(p)q^2 + f_1(p); \quad (5.12)$$
$$d_1(p) = -2p\Im \{ \varepsilon^* \varepsilon_2 \} + |\varepsilon^* - \varepsilon_2|^2 \Im \{ \theta \},$$
$$e_1(p) = 2p^2\Im \{ \varepsilon^* \varepsilon_2 \} - 2p\Im \{ (\varepsilon^* - \varepsilon_2)\varepsilon_2\varepsilon_2\theta \} + |\varepsilon^* - \varepsilon_2|^2 \Im \{ \theta^2 \},$$
$$f_1(p) = 2p^3\Im \{ (\varepsilon^* + \varepsilon_2)\varepsilon_2\varepsilon_2\theta \} + 2p\Im \{ (\varepsilon^* - \varepsilon_2)\varepsilon_2\varepsilon_2\theta^2 \} - 2p|\theta|^2 \Im \{ \varepsilon^* \varepsilon_2 \} + |\theta|^2 |\varepsilon^* - \varepsilon_2|^2 \Im \{ \theta \}.$$
(d.2) Inverting the second arc of \( \mathcal{R}_2^{mp} \)

Inverting \( T_{2,2}(z; p, q) \) gives \( G_{2,2}(p, q) = a_2(q)p^2 + b_2(q)p + c_2(q) \) with

\[
\begin{align*}
a_2(q) &= 2 \Im \left\{ [\varepsilon^*(\theta + q^2) + \varepsilon_2(\theta - q^2)] e^* \right\}, \\
b_2(q) &= 2 \Re \left\{ (\varepsilon^* - \varepsilon_2)(\theta^2 - q^2)e^* \right\} \\
&\quad + 3 \left\{ [\varepsilon^*(\theta + q^2) + \varepsilon_2(\theta - q^2)] (\varepsilon^* - \varepsilon_2)(\theta - q^2) \right\}, \\
c_2(q) &= |q - \theta|^2|\varepsilon^* - \varepsilon_2|^2 \Im \{\theta\}.
\end{align*}
\]

The algebraic curve \( G_{2,2}(p, q) = 0 \) is given by

\[
p = \frac{-b_2(q) \pm \sqrt{[b_2(q)]^2 - 4a_2(q)c_2(q)}}{2a_2(q)}.
\]

(5.13)

Both roots appear in the full display of the curve on the right side of figure 2.

(e) Matching forward and inverse regions

The curves \( G_{i,j}(p, q) = 0 \) are boundary curves; it remains to determine which side of the boundaries the admissible parameter values lie. When \( q = 1 \), \( \mathcal{R}_1^{mp} \) reduces to \( \mathcal{R}_1 \) so that the inverse region determined by \( \mathcal{R}_1^{mp} \) must contain the line segment \([p_{1,1}, 1], (p_{1,\infty}, 1)] \). Similarly, the inverse region determined by \( \mathcal{R}_2^{mp} \) must contain the shorter segment \([p_{2,1}, 1], (p_{2,\infty}, 1)] \). A complete matching the forward regions with the corresponding inverse regions may be done by computing forward regions at selected \((p, q)\) pairs. Figure 3 illustrates this process.

(f) If \( F_\zeta(\pi) = 0 \) has no real roots.

We return to a discussion of the inversion algorithm in general, not just its application to sea ice. We follow the same notation of Theorem 1 and again consider \( \pi_1, \ldots, \pi_n \) as variable (real) parameters.

It may happen that \( F_\zeta(\pi) = F_\zeta(\pi_1, \ldots, \pi_n) = 0 \) has no real roots. The following theorem addresses this issue. Here is its practical application: suppose for an observed effective property \( \zeta \in \mathbb{C} \) we have \( F_\zeta(\pi) \neq 0 \) for all relevant parameter values \( \pi \). According to Theorem 1 this means that the circles \( T_\pi(\mathbb{R}) \) do not come into contact with \( \zeta \) as \( \pi \) varies. Theorem 2 gives criteria to decide if this is because \( \zeta \) always lies inside, or always lies outside, each of the circles \( T_\pi(\mathbb{R}) \).

The new notation \( \Lambda_n \), denoting a subset of \( \mathbb{R}^n \), accounts for the fact that relevant parameter values may not comprise all of \( \mathbb{R}^n \). For example, for our sea ice problem, the relevant values of \((p, q)\) lie in \( \Lambda_2 = [0, 1] \times [0, 1] \subseteq \mathbb{R}^2 \). We also introduce the notation \( \Lambda_n' \) denoting a connected subset of \( \Lambda_n \). In most applications we would expect \( \Lambda_n' = \Lambda_n \). Jones & Singerman (1987, p. 28) discuss the ‘circle inversion’ mentioned after (5.16).
Theorem 2. Suppose $\Lambda_n'$ is a connected subset of parameter set $\Lambda_n \subseteq \mathbb{R}^n$ and
\[ \Im\{\overline{C(\pi)}D(\pi)\} \neq 0 \quad \forall \pi = (\pi_1, \ldots, \pi_n) \in \Lambda_n'. \quad (5.14) \]
If $F_\zeta(\pi) = 0$ has no real roots then $\zeta$ lies outside each circle in the family $\{T_\pi(\mathbb{R}) : \pi \in \Lambda_n'\}$ provided the following inequality holds for at least one $\pi \in \Lambda_n'$:
\[ \left| \zeta - \frac{i}{2} \frac{A(\pi)D(\pi) - B(\pi)C(\pi)}{\Im\{C(\pi)D(\pi)\}} \right| > \frac{1}{2} \frac{|A(\pi)D(\pi) - B(\pi)C(\pi)|}{\Im\{C(\pi)D(\pi)\}}. \quad (5.15) \]

If $F_\zeta(\pi) = 0$ has no real roots then $\zeta$ lies inside each circle in $\{T_\pi(\mathbb{R}) : \pi \in \Lambda_n'\}$ provided that the reverse inequality in (5.15) holds for at least one $\pi \in \Lambda_n'$.

Proof. First, the hypothesis (5.14) implies that each $T_\pi(\mathbb{R})$ is a circle of finite radius. Otherwise, $T_\pi(\mathbb{R} \cup \{\infty\})$ would be a straight line in $\mathbb{C}$ passing through $\infty$ in the extended complex plane, implying that $T_\pi(z) = \infty$ for some $z \in \mathbb{R} \cup \{\infty\}$. Upon computing $z = T_\pi^{-1}(\infty)$, we find $z = -D(\pi)/C(\pi) \notin R$ by (5.14), and $-D(\pi)/C(\pi) \neq \infty$ also by (5.14). Therefore $T_\pi(\mathbb{R})$ has finite radius.

Next, let $\xi(\pi)$ and $\rho(\pi)$ denote the center and radius of $T_\pi(\mathbb{R})$ respectively:
\[ \xi(\pi) = \frac{i}{2} \frac{A(\pi)D(\pi) - B(\pi)C(\pi)}{\Im\{C(\pi)D(\pi)\}}, \quad \rho(\pi) = \frac{1}{2} \frac{|A(\pi)D(\pi) - B(\pi)C(\pi)|}{\Im\{C(\pi)D(\pi)\}}. \quad (5.16) \]
These may be derived by noting that inversion in the circle $T_\pi(\mathbb{R})$ exchanges $\xi$ and $\infty$, and is conjugate via $T_\pi$ to a reflection across $R$. Since $\infty = T_\pi(-D(\pi)/C(\pi))$ it follows that $\xi(\pi) = T_\pi(-D(\pi)/C(\pi))$ yielding the indicated formula; and $\rho(\pi) = |\xi(\pi) - T_\pi(\infty)|$. Formulas (5.16) show that $\xi(\pi)$ and $\rho(\pi)$ are continuous.

Define $J : \Lambda_n' \rightarrow \mathbb{R}$ by $J(\pi) = |\xi(\pi) - \xi(\pi)| - \rho(\pi)$. Note that $0 \notin J(\Lambda_n')$. (Otherwise $\zeta \in T_\pi(\mathbb{R})$ for some $\pi \in \Lambda_n'$ and then $F_\zeta(\pi) = 0$ would have a real root in $\Lambda_n'$ by Theorem 1.) Since $J$ is continuous, $J(\Lambda_n')$ is connected. Hence either $J(\pi) > 0$ for all $\pi \in \Lambda_n'$ or $J(\pi) < 0$ for all $\pi \in \Lambda_n'$. If (5.15) holds for a particular $\pi^* \in \Lambda_n'$ then $J(\pi^*) > 0$, hence $J(\pi) > 0$ for all $\pi \in \Lambda_n'$, so that $\zeta$ lies outside each circle $T_\pi(\mathbb{R})$ for all $\pi \in \Lambda_n'$. Similar reasoning handles the reverse inequality in (5.15).

Theorem 2 has the following corollary in its specialization to sea ice: if for
a given $\varepsilon^* \neq 0$, $F_{i,j}(p)$ fails to have a real root, then $\varepsilon^*$ lies outside the circles $T_{i,j}(\mathbb{R}; p)$ for all $p \in [0,1]$; if for a given $\varepsilon^* \neq 0$, $G_{i,j}(p, q)$ fails to have a real root then $\varepsilon^*$ lies outside the circle $T_{i,j}(\mathbb{R}; p, q)$ for all $(p, q) \in [0,1] \times [0,1]$. This is because for each entry on the right hand side of table 1 there exists a $p \in [0,1]$ such that $A(p)D(p) - B(p)C(p) = 0$; and for each entry on the right hand side of table 2 there exists a $(p, q) \in [0,1] \times [0,1]$, such that $A(p, q)D(p, q) - B(p, q)C(p, q) = 0$.

6. Inverse bounds for volume fraction

In this section we consider the problem of inverting for the single parameter $p$ before considering both $p$ and $q$ in §7. We apply the inversion method developed in §5 is to obtain upper and lower bounds on $p$ using the effective complex permittivity data for sea ice given in table 5. We then compare these bounds
Figure 3. Matching forward and inverse regions. The top left figure reproduces figure 2 and shows $(p, q)$ pairs selected at point 1 (.017, .992), point 2 (.017, .927), and point 3 (.009, .979). The same observed $\varepsilon^* = 3.24 + 0.08i$ is shown in the three panels depicting forward regions. Point 1 yields regions $R_1, R_2, R_{1mp}$, and $R_{2mp}$ all of which cover $\varepsilon^*$. For point 2, $R_1$ and $R_2$ cover $\varepsilon^*$ while $R_{1mp}$ and $R_{2mp}$ do not. For point 3, $R_1$ and $R_{1mp}$ cover $\varepsilon^*$ but $R_2$ and $R_{2mp}$ do not. Data are given in table 6.

with an empirical formula from Frankenstein & Garner (1967) that determines brine volume from temperature and salinity.

The inversion formulas for $\hat{p}_{1, \ell}, \hat{p}_{1, u}, \hat{p}_{2, \ell}, \hat{p}_{2, u}$ depend on $\varepsilon^*$, and the complex permittivities of the two phases, $\varepsilon_1$ and $\varepsilon_2$. The latter two may be calculated from the measured temperature, sample salinity, sample density, and the electromagnetic frequency of the experiments, using the formulae described next.

Concerning $\varepsilon_1$, the complex permittivity of the brine, we use the calculations of Stogryn & Desargant (1985) that are based on a Debye-type relaxation equation,

$$
\varepsilon_1 = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - i2\pi f \tau} + i \frac{\sigma}{2\pi \varepsilon_0 f}, \quad i = \sqrt{-1},
$$

(6.1)
in which $f$ denotes the frequency in GHz, and $\varepsilon_\infty, \varepsilon_s, \tau$, and $\sigma$ are expressed as functions of temperature by the following equations fit to experimental data:

$$
\varepsilon_\infty = \frac{82.79 + 8.19T^2}{15.68 + T^2}, \quad \varepsilon_s = \frac{939.66 - 19.068T}{10.737 - T},
$$

$$
2\pi\tau = 0.10990 + 0.13603 \times 10^{-2}T + 0.20894 \times 10^{-3}T^2 + 0.28167 \times 10^{-5}T^3,
$$

$$
\sigma = \begin{cases} 
-T \exp[0.5193 + .08755T] & \text{if } T \geq -22.9^\circ\text{C}, \\
-T \exp[1.0334 + .1100T] & \text{if } T \leq -22.9^\circ\text{C}.
\end{cases}
$$

Here $\varepsilon_s$ and $\varepsilon_\infty$ are the limiting static and high frequency values of the real part of $\varepsilon_1$, $\tau$ is the relaxation time in nanoseconds, $\varepsilon_0$ is the permittivity of free space, $8.85419 \times 10^{-12} \text{F/cm}$, and $\sigma$ is the ionic conductivity of the dissolved salts in siemens per metre. It is assumed that $\sigma$ is independent of frequency.

### Table 3. Coefficients of $F_1(T)$ and $F_2(T)$ for $-22.9^\circ\text{C} \leq T \leq -2^\circ\text{C}$ (Cox & Weeks 1983, p. 312).

<table>
<thead>
<tr>
<th>$F_1(T)$</th>
<th>$F_2(T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_0$</td>
<td>$-4.732$</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>$-2.245 \times 10^1$</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>$-6.379 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\alpha_3$</td>
<td>$-1.074 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Concerning $\varepsilon_2$, it was found by Cherkaeva & Golden (1998) that the theoretical forward bounds fit the data more closely by accounting for air in the sea ice. In particular, the complex permittivity of the ice $\varepsilon_2$ was calculated as a permittivity of a composite with a small volume fraction of air using the Maxwell–Garnett formula. We use the same approach here:

$$
\varepsilon_2 = \varepsilon_{\text{ice}} \left[ 1 - \frac{d p_{\text{air}}(\varepsilon_{\text{ice}} - \varepsilon_{\text{air}})}{\varepsilon_{\text{ice}}(d - 1) + \varepsilon_{\text{air}} + p_{\text{air}}(\varepsilon_{\text{ice}} - \varepsilon_{\text{air}})} \right], \quad (6.2)
$$

Here $\varepsilon_{\text{ice}} = (3.1884 + .00091T) + .00005i$ (Matzler & Wegmuller 1987, 1988), $\varepsilon_{\text{air}} = 1$, and the volume fraction of air, $p_{\text{air}}$, is calculated via the equations given by Cox & Weeks (1983):

$$
p_{\text{air}} = \frac{V_{\text{air}}}{V} = 1 - \frac{\rho}{\rho_{\text{ice}}} + \rho S \frac{F_2(T)}{F_1(T)}.
$$

Here $\rho$ is the density of the sea ice sample in g/cm$^3$; $T$ is its temperature in °C; $S$ is its salinity in ppt; and $\rho_{\text{ice}}$ is the density of pure ice in g/cm$^3$, which is given by $\rho_{\text{ice}} = 0.917 - 1.403 \times 10^{-4}T$; and the coefficients of $F_j(T) = \alpha_0 + \alpha_1 T + \alpha_2 T^2 + \alpha_3 T^3$, $j = 1, 2$ are given in table 3. In (6.2) we take $d = 3$, as the air inclusions in actual sea ice are uniformly and isotropically distributed throughout the ice in three dimensions, as opposed to the brine inclusions.

Table 4 and figure 4 compare the result of inverting for brine volume fraction from effective complex permittivity with the result of computing brine volume.
fraction using the equation of Frankenstein & Garner (1967):

\[ p = p_1 = \begin{cases} 
0.001 \ S (43.795 |T|^{-1} + 1.189) & -22.9 \leq T \leq -8.2, \\
0.001 \ S (45.917 |T|^{-1} + 0.930) & -8.2 \leq T \leq -2.06, \\
0.001 \ S (52.56 |T|^{-1} - 2.28) & -2.06 \leq T \leq -0.5. 
\] (6.3)

Here \( T \) is the temperature in °C and \( S \) is the salinity in parts per thousand.

7. Inverse bounds for inclusion separation

Figure 2 shows typical inverse bounds on \( p \) and \( q \). For a given brine volume fraction \( \hat{p}_2,\ell \leq p \leq \hat{p}_2,u \) we may determine an interval of admissible \( q \) values from the second order matrix particle bounds: it is the interval \( q_{\text{min}}(\hat{p}_2) \leq q \leq 1 \), where \( q_{\text{min}}(\hat{p}_2) \) is the value of \( q \) where a horizontal line at level \( \hat{p}_2 \) will intersect the inverse boundary curve from the first arc of \( R_{1/2}^{mp} \). Thus \( q_{\text{min}}(\hat{p}_2) \) may be computed by setting (5.12) equal to zero and solving for \( q \):

\[ q_{\text{min}}(\hat{p}_2) = -e_1(\hat{p}_2) - \sqrt{\left[e_1(\hat{p}_2) - 4d_1(\hat{p}_2)f_1(\hat{p}_2)\right]^2 - 4d_1(\hat{p}_2)f_1(\hat{p}_2)}, \quad \hat{p}_2,\ell \leq p \leq \hat{p}_2,u. \] (7.1)

If \( p \) is not in the indicated interval, then we set \( q_{\text{min}}(\hat{p}_2) = 1 \). Here \( d_1(p) \), \( e_1(p) \), and \( f_1(p) \) are given by (5.12). The need for the minus sign on the square root was established numerically.

Figure 5 shows \( q_{\text{min}}(p_c) \) calculated by (7.1), with \( p_c \) calculated by (6.3), using data given in table 5. It indicates a coalescence toward percolation as the temperature rises. Since 1 is always the upper bound, we can not make inferences about the ice being bounded away from percolation, at colder temperatures. Nevertheless the lower bound \( q_{\text{min}}(p) \) is still informative; it bounds \( q \) toward percolation.
Table 4. Inverse bounds for laboratory ice slab data: complex permittivity data from table 5 are used to compute bounds $\hat{\varepsilon}_1, \ell, \hat{\varepsilon}_1, u, \hat{\varepsilon}_2, \ell, \hat{\varepsilon}_2, u$ using (5.7–5.10) with $\varepsilon_1$ and $\varepsilon_2$ determined using (6.1) and (6.2) respectively. The column labeled $\hat{\rho}_c$ gives the brine volume fractions computed using (6.3) from which $q_{\text{min}}(\hat{\rho}_c)$ is computed using (7.1). The complete table is in the electronic supplementary material. Notes: (a) the value for $\hat{\rho}_2$ computed by solving $F_2(\rho) = 0$ is complex hence theorem 2 is applicable: the observed effective complex permittivity lies outside the forward bounds for all parameter values $\rho \in [0,1]$; (b) $T = -27.0^\circ\text{C}$ lies outside the range given in (6.3); (c) the value $q_{\text{min}}(\rho_c) = 1$ occurs because $\rho_c > \hat{\rho}_2,u$, which can also be seen in figure 4.

<table>
<thead>
<tr>
<th>Slab</th>
<th>$^\circ\text{C}$</th>
<th>$\hat{\rho}_1,\ell$</th>
<th>$\hat{\rho}_1,u$</th>
<th>$\hat{\rho}_2,\ell$</th>
<th>$\hat{\rho}_2,u$</th>
<th>$\rho_c$</th>
<th>$q_{\text{min}}(\rho_c)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>84-3</td>
<td>-22.5</td>
<td>-0.2352</td>
<td>0.0088</td>
<td>(a)</td>
<td>0.0047</td>
<td>0.0119</td>
<td>--</td>
</tr>
<tr>
<td></td>
<td>-20.0</td>
<td>0.0078</td>
<td>0.0415</td>
<td>0.0124</td>
<td>0.0250</td>
<td>0.0128</td>
<td>0.9383</td>
</tr>
<tr>
<td></td>
<td>-18.0</td>
<td>0.0074</td>
<td>0.0415</td>
<td>0.0119</td>
<td>0.0249</td>
<td>0.0138</td>
<td>0.9466</td>
</tr>
<tr>
<td></td>
<td>-17.5</td>
<td>0.0084</td>
<td>0.0458</td>
<td>0.0132</td>
<td>0.0270</td>
<td>0.0140</td>
<td>0.9308</td>
</tr>
<tr>
<td></td>
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<td>0.0251</td>
<td>0.1545</td>
<td>0.0418</td>
<td>0.0956</td>
<td>0.1245</td>
<td>1 (c)</td>
</tr>
<tr>
<td>84-4</td>
<td>-27.0</td>
<td>-2.8138</td>
<td>0.0285</td>
<td>(a)</td>
<td>0.0154</td>
<td>(b)</td>
<td>--</td>
</tr>
<tr>
<td></td>
<td>-22.0</td>
<td>0.0020</td>
<td>0.0082</td>
<td>0.0035</td>
<td>0.0059</td>
<td>0.0121</td>
<td>1 (c)</td>
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<tr>
<td></td>
<td>-20.5</td>
<td>0.0062</td>
<td>0.0335</td>
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<td>0.0209</td>
<td>0.0126</td>
<td>0.9626</td>
</tr>
<tr>
<td></td>
<td>-10.0</td>
<td>0.0071</td>
<td>0.0459</td>
<td>0.0119</td>
<td>0.0275</td>
<td>0.0212</td>
<td>0.9814</td>
</tr>
<tr>
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<td>-9.0</td>
<td>0.0055</td>
<td>0.0296</td>
<td>0.0098</td>
<td>0.0198</td>
<td>0.0230</td>
<td>1 (c)</td>
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<tr>
<td></td>
<td>-7.5</td>
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<td>0.0268</td>
<td>1 (c)</td>
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<td>0.0326</td>
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<tr>
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<td>0.1502</td>
<td>0.0414</td>
<td>0.0943</td>
<td>0.0912</td>
<td>0.9979</td>
</tr>
</tbody>
</table>

8. Data

Tables 5 and 6 record data used herein; see also electronic supplementary material.

Acknowledgment

We gratefully acknowledge grant support from the Division of Mathematical Sciences (DMS-0940249) and Office of Polar Programs (ARC-0934721) at the US National Science Foundation.

References


Figure 5. Slab temperature versus minimum separation parameter $q_{\text{min}}(p_c)$. The latter is computed by (7.1) using only those values of $p_c$ computed by (6.3) that lie between $\hat{p}_2,\ell$ and $\hat{p}_2,u$. Data are from the first and last columns of table 4. The inverted data displayed here illustrate that as the ice warms, the separations of the brine inclusions decrease. It is significant that this important phenomenon is being characterized electromagnetically through an inversion scheme. (Online version in color.)

Table 5. Laboratory ice slab data from Arcone et al. (1986, figure 7, p. 14,289) are the real and imaginary parts of $\varepsilon^*$ measured with waves vertically incident to the slabs at 4.75 GHz. Slab 84-3 has salinity 3.8 ppt, density 0.884 g/cm$^3$. Slab 84-4 has salinity 3.8 ppt, density 0.886 g/cm$^3$. The complete table, containing measurements of both slabs, is in the electronic supplementary material.

<table>
<thead>
<tr>
<th>Table 5</th>
<th>Slab 84-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(°C)</td>
<td>-27.0 -22.0 -20.5 -19.5 -18.0 -16.5</td>
</tr>
<tr>
<td>Im$\varepsilon^*$</td>
<td>0 0.048 0.089 0.077 0.089 0.089</td>
</tr>
</tbody>
</table>

| (°C)    | -9.0 -7.5 -6.0 -5.5 -4.5 -3.5 | -2.5 -2.0 |
| Re$\varepsilon^*$ | 3.289 3.333 3.504 3.548 3.585 3.719 | 3.822 4.000 |
| Im$\varepsilon^*$ | 0.155 0.173 0.238 0.254 0.258 0.250 | 0.280 0.315 |

Table 6. Data used in figures 1, 2, and 3 (Golden et al. 1998, Arcone et al. 1986).

<table>
<thead>
<tr>
<th>$\varepsilon_1$</th>
<th>$\varepsilon_2$</th>
<th>$\varepsilon^*$</th>
<th>frequency</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>33.30 + 39.89i</td>
<td>3.068 + 0.00006i</td>
<td>3.24 + 0.08i</td>
<td>4.75 GHz</td>
<td>-18.5 °C</td>
</tr>
</tbody>
</table>


