Localization and Transport Effects in the Disordered Materials

Vladislav Malyshkin
Western Michigan University
LOCALIZATION AND TRANSPORT EFFECTS
IN THE DISORDERED MATERIALS

by
Vladislav Malyshkin

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We study the thermal conductivity due to vibrational waves of an amorphous network of atoms, the optical transmissivity of random optical systems, and the speckle correlations and inverse scattering problem in optical surface physics. The thermal conductivity study was performed by modeling an amorphous material as an fcc percolating cluster of atoms. Unlike previous scalar wave treatments of the atomic vibrations, in the current model we considered full 3D motions of the atoms. Two different phonon scattering mechanism were considered: scattering from the random network (network scattering) and scattering accompanied by changes in the network geometry (two level states model). Our results exhibit the three regions of different temperature dependent behavior observed experimentally for \( T \leq 100K \). The thermal conductivity in the plateau region \( 1K < T < 10K \) and its lower temperature limit are dominated by Rayleigh scattering from the amorphous network. The exponent \( \beta \) in the low-temperature limit \( T < 1K \) of the thermal conductivity \( (K \propto T^\beta) \) was determined to be in the range \( 1 \leq \beta \leq 2 \).

In a second project we studied the strong transverse localization of light in 1D and 2D optical systems. A strong polarization dependence was found in both 1D and 2D cases.

In a third project we studied the inverse problem in optical scattering from 1D randomly rough metal surface. From the experimentally measured dif-
ferential reflection coefficient we determined the statistics of the surface profile. We employed a Reverse Monte Carlo approach similar to that introduced for the processing of X-ray scattering data from polymers and amorphous materials and extracting the statistical properties related to the atomic positions in these materials.

In a fourth project we studied the speckle correlations in the case of optical scattering from 1D randomly rough metal surface. We did this by using diagrammatic perturbation theory and computer simulations. Several new correlations were predicted. Some of these correlations were shown to be related to the resonant excitation of the surface electromagnetic waves (surface plasmon polaritons). These correlations were found to give important information about surface electromagnetic waves and the surface structure of the randomly rough metal surfaces.
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Vladislav Malyshkin
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CHAPTER I

INTRODUCTION

In this dissertation we study some general properties of acoustical and optical disordered systems. We will be concerned with computing some transport properties in these systems and also in using scattering in these system to determine the system structure and the nature of the system excitations.

Specifically, we will study the thermal conductivity of an amorphous network, the optical transmisivity of random optical systems, and the speckle correlations and inverse scattering problem in optical surface physics. In the thermal conductivity problem and optical transmisivity we will be interested in the nature of propagating and Anderson localized states. In the speckle and inverse optical problem we will be interested in the determination of the surface structure and excitations associated with the scattering of light from rough metal surfaces. We will first give an overview of the effects of disorder on the excitations in a system and then we will provide an overview of our four related projects.

Disorder is very important in determining the transport properties (e.g. heat conductivity and optical energy flow) in acoustic and optical systems and as such it is necessary to understand as a guide to technological application of acoustical and optical materials. Different phenomena exhibited in optical and acoustical systems depend on the strength and nature of the disorder as this strength of disorder directly affects the wavefunctions of the excitations in these systems. Specifically, some types of disorder give rise to systems with non-zero transport
characteristics while other types of disorder give rise to Anderson localization and systems which do not support transport (zero transport coefficients). Hence a knowledge of the conditions which give rise to Anderson localization is necessary to completely understand the nature of transport in disordered materials.

In this dissertation we study disordered vibrational and optical systems which exhibit both localized and nonlocalized excitations. We shall be interested in how localized and non-localized states can be identified and in the identification of their effects on the physical properties of these systems. Specifically, in amorphous insulating solids the heat transfer by lattice vibrations depends on the diffusive (non-localized) modes of the system, which are scattered by the random network geometry. In addition, we shall examine localization effects in the random optical systems in which it is found to inhibit light or energy propagation. Finally we shall examine the scattering of light from rough surfaces and determine how Anderson localized surface electromagnetic waves can be observed in the speckle correlations of light scattered from rough metal surfaces.

Localization is one of the most interesting effects studied in the physics of disordered materials. It has been observed experimentally in electronic (see Ref. [27] for a good review), acoustic, optical, magnetic and other miscellaneous systems. Specifically, localization arises when the wave function amplitudes of the excitations in a system are essentially not zero only in some small region of space. The localization effect can be caused by a number of different mechanisms. A typical mechanism is random disorder which is a basic source of localization in many systems, but even in systems without any disorder localization can be caused by non-linear or interference effects. Localized states do not contribute to diffusive processes which give rise to transport coefficients so it is important to
know how they arise and their affect on the overall value of computed transport coefficient.

Disorder usually exists in varying degrees in any physical system and its ability to produce localized states depends on the strength and dimensionality of the system. Specifically in 3D systems only strong disorder can cause localization, but in 2D and 1D systems any disorder (no matter how weak) causes localization. The weak 3D disorder limit is traditionally described by the scattering of Bloch waves by impurities. Such processes contribute to the measured non zero transport properties of these systems and many theories have been put forth in order to explain such effects. In the strong disorder 3D systems one can suppose that because of the random potential the wave function may be profoundly altered if the randomness is sufficiently strong. The traditional view had been that scattering by the random potential causes the Bloch wave to loose phase coherence on the length scale of the mean free path $l$, but nevertheless the wave function is extended through the sample. Anderson [1] pointed out that if the disorder is very strong, the wave function may become localized and decay exponentially from some point in space $\propto \exp(|r - r_0|/\xi)$ where $\xi$ is the localization length. This is very clear in the limit of very strong disorder. The zeroth order description of the eigenstate would be a bound state or a localized orbital bound by deep fluctuation in the random potential. Then we could consider the admixture between different fluctuations as a perturbation. This will not produce an extended state because the wave functions that overlap significantly are in general very different in energy and states that are nearly degenerated are in general very far apart in space. So in the very strong disorder limit the wave functions are exponentially localized. In the one dimensional case Mott and Twose [41], and Borland [8] have proved
that all states are localized, no matter how weak the disorder. Later Anderson showed that in the 2D case all states are also localized, no matter how weak the disorder. Consequently, 1D and 2D systems in the presence or disorder are very useful systems in which to investigate localization.

The weak 3D and strong 3D, 2D and 1D disorder limits are more or less well understood but the intermediate 3D and weak 2D and 1D disorder cases are not so well understood. It is only with the development of high speed computers that an essential amount of progress can be achieved in the intermediate disorder effects and weak effects in 2D and 1D systems.

Phase coherent effects similar to those which give rise to Anderson Localization can be observed in optical systems as well. The enhanced backscattering of light from rough metal surfaces is related to the presence of two related types of “trajectories” of light propagation in the scattering from the rough surfaces. These are the direct “trajectory” and the time-reverse of the direct “trajectory”. When the incident direction is the same as the final scattered direction these two “trajectories” give constructive interference and a retroreflection peak in the differential reflection coefficient. In three dimensional electrons, acoustic and optical systems these phase coherent scattering trajectories give rise to enhanced backscattering which create Anderson localized states. In our study of speckle correlation we shall find similar phase coherent interference effects as discussed above and these are found to lead to a number of peaks in the speckle correlator. These peaks allow us to obtain information about electromagnetic wave modes in the random media and their Anderson localization properties.

We now give an overview of the thermal conductivity and random optical system projects to be discussed in the dissertation. These are related to transport
characteristics. This will be followed by a discussion of surface optics projects which are related to the localization of surface waves and the determination of surface properties from the resonant scattering from surface wave excitation.

First we study diffusive behavior in acoustical systems. We perform computer simulation studies of the heat conductivity of amorphous insulating solids. Heat transfer in this system is by lattice vibrational excitations and these excitations are scattered by the disorder of the amorphous network. The non-localized vibrational states give the most important contribution to heat transfer. Localization in the system in question is not very significant because of the hopping between different localizes states that take place at finite temperature. The non zero heat conductivity depends solely on the diffusivity of phonon modes and on the density of states (the number of phonon modes per given frequency interval). The phonon diffusivity has two contributions. The first one is due to scattering accompanied by transitions between different metastable network configurations. This contribution only exist in amorphous materials. We use a phenomenological theory (two level states theory) developed by Anderson et al [2] and Philips [50] to describe such processes. The second contribution is due to the scattering by the disorder of the fixed network geometry in the system existent in one unchanging metastable state. We studied it by performing a numerical diffusion experiment for pulse spreading in the system. The density of vibrational states is then calculated by using the recursion technique developed by Haydock et al [16]. Combining the diffusivity, density of vibrational states and the two level states theory allows us to compute the heat conductivity. Our results are in reasonable agreement with experimental measurements made on amorphous materials.

In the second part of this work we will study localization in bulk optical
systems in which disorder is the basic cause of localization.

In this dissertation we study localization effects in the 1D and 2D optical systems. We start with studies on a 1D system. The system is a layered system of slabs separated by vacuum. The slab widths and the distance between slabs are fluctuating randomly. For electric field calculations we used the transfer matrix approach developed in [69] and compute the localization properties of electromagnetic beams as a function of the incident angle measured relative to the normal to the slab surface. Important differences are observed in the localization properties of the two different polarizations of electromagnetic waves in the system. We find that in 1D systems s polarized waves are easier localized than p polarization. This corresponds to the result obtained in Ref. [55] for plane waves that p polarization is never localized if the incident wave is incident at the Brewster angle.

We next study 2D optical systems. These systems contains a number of square rods with a background fluctuating dielectric constant. Usually it is very hard to calculate the localization length in 2D systems directly. Because of that we performed the following procedure. We study many periodic systems with identical unit cells in each system, but for each new system we take the new unit cell. So we have a set of periodic systems with different unit cells in each system. We used a numerical integration approach due to Pendry *et al* [6] to calculate the electric field in the given periodic system. After performing configuration averaging, we can get the localization length as a function of disorder in the system with the different cells (this is correct only if the localization length is less or about the unit cell size). We study the 2D systems for two polarizations and for a number of incident angles. Interesting localization behaviors are found which exhibit polarization dependence and dependence on the angle of incidence.
Another topic of interest to us is the characterization of surface and surface excitations by light scattering. Specifically, in a third project, we study a randomly rough metal surface and used a new reverse Monte Carlo method for the determination of the surface profile statistics from measured differential reflection data for the scattering of electromagnetic radiation. The Reverse Monte Carlo (RMC) technique has recently been developed in material science where it has been applied to the determination of the structures of amorphous and polymer materials from X-ray scattering data [36]. This method uses Monte Carlo and maximum entropy technique to generate atomic structures which reproduce the scattering data obtained experimentally from disordered systems. This generated atomic structures then act as models for the atomic arrangement in the materials. We used this method to extract the power spectrum of a randomly rough surface from the differential reflection coefficient of electromagnetic radiation scattered from such a surface, i.e. from far-field experimental data. Excellent agreement with the power spectrum data obtained from contact profilometry methods is observed.

In a fourth project we studied the speckle correlations of light multiply scattered from the randomly rough metal surfaces. To calculate the scattered electromagnetic field we used the perturbation theory from Ref. [35]. This theory gives us $H(q, k)$ (the amplitude of the magnetic field with scattered wave vector $q$ for an incident wave with incident wave vector component parallel to the mean surface $k$). Most of the previous studies (see Ref. [9] for a review) were made in the context of a first order perturbation theory or Kirchhoff approximation treatment of the scattering of light. In contrast with these studies that are equivalent to a single scattering approach, the theory from Ref. [35] is correct to the second order
to the surface profile. It takes into account double scattering from the surface and displays enhanced backscattering from the surface.

While the differential reflection coefficient has been extensively studied for several decades, the subject of the intensity correlations in the scattering of electromagnetic waves from randomly rough surfaces has become significant only in the last several years. When incident light scatters from a randomly rough surface, we obtain speckle structure in the intensity of scattered light. When we change the angle of incidence of the light the speckle structure changes. The correlation in the intensity between different speckle patterns is the subject of study in the fourth project. In earlier studies [13,22,40,45,47] speckle patterns were studied theoretically in the single scattering approximation. The correlations that are due to the multiple scattering effects have only recently begun to be considered Ref. [3,25,28,46] in bulk scattering. Such kind of multiple scattering have led to the prediction of a number of novel features in the bulk scattered light, some of which have been observed experimentally [25,28]. We shall be interested in multiple scattering effects in speckle patterns.

The best known speckle correlation effect for light scattered by bulk and surface scattering surfaces is the memory effect (strong peak in the speckle correlations at $q - k = q' - k'$, where $k$ and $k'$ are the wave vector components parallel to the mean surface of two incident waves and $q$ and $q'$ are the wavevector components parallel to the mean surface for the scattered waves). In our studies we find new effects which are not related to the memory effect or to the multiple scattering effect previously observed in bulk of surface scattering. These effects which occur in higher order of perturbation theory than the memory effects include new peaks associated with the surface electromagnetic excitations.
In our studies of the speckle correlations from the randomly rough surface we used the following procedure. First we numerically generated a randomly rough surface by using the approach of Ref. [34]. Next we calculated the scattered field for light incident on the rough surface by using multiple scattering [35] theory. Then we performed a configuration averaging of \( I(q, k) \), \( I(q', k') \) and \( I(q, k)I(q', k') \) over ensemble of the random surfaces and obtained the speckle correlations \( C = \langle I(q, k)I(q', k') \rangle - \langle I(q, k) \rangle \langle I(q', k') \rangle \). The well known memory effect is observed as well as several new high-order peaks (these peaks are due to the surface plasmon-polariton excitations) are obtained. These new lines are present only in the case of multiple scattering and are absent in the single scattering approximation.

We begin Chapter II with an introduction to the thermal conductivity study. In Section II.2 we will discuss the relationship between the thermal conductivity and the density of vibrational states, the specific heat and the diffusivity of vibrational waves as a function of vibrational wave frequency in an amorphous solid. A model will be presented which will be used to perform computer simulation studies of the density of vibrational modes in frequency and the frequency dependent diffusion constant in a fixed random network. (The phenomenological two level states theory will be used to treat those contribution to the total diffusion constant which arise from scattering accompanying change in the geometry of the random network.) In Section II.3, we discuss the computation using the recursive methods of the density of vibrational modes in frequency of our model amorphous system. In contrast to past simulation efforts, the present simulation allows for full three dimensional motion of the atoms, and exhibits results for the thermal conductivity and density of states of the vibrational modes which differ...
from previous simulation results [58]. In Section II.4, the computation of the diffusion coefficient is discussed for both types of scattering mechanisms mentioned above. In Section II.5, the results of Sections II.3 and II.4 are used to compute the thermal conductivity and our conclusions are presented in Section II.6.

In Chapter III we study localization in one- and two-dimensional optical systems. We study a random system of dielectric slabs separated by vacuum. In Section III.1 we describe our system and write down the boundary conditions. In Section III.3 we discuss application of the transfer matrix method to study the system. In the Section III.5 we calculate the localization properties and present a discussion of results. In Chapter III.9 we present a summary and conclusion.

In Chapter IV we study the determination of the surface profile statistics from the optical scattering data. In Section IV.1 we give some introduction to the Reverse Monte Carlo (RMC) method and discuss an application of the RMC method to the determination of the surface profile to experimental data by West and O'Donnell [67] and make comparison with surface profile results obtained using contact surface profilometry. In Section IV.2 we discuss the obtained results.

In Chapter V we study the speckle correlations of light multiply scattered from the randomly rough metal surfaces. In Section V.1 we give some introduction and discuss the result of the other authors. Then in Section V.2 we present the diagrammatic perturbation theory we used to calculate the properties of scattered light. In Section V.3 we present obtained results. In Section V.4 we perform direct numerical simulation for the scattered light and compare obtained results with those in Section V.3.

In Chapter VI we present a summary and conclusion.
CHAPTER II

COMPUTER SIMULATION STUDY OF THE THERMAL CONDUCTIVITY OF AMORPHOUS INSULATING SOLIDS

II.1. Introduction

Amorphous insulating solids in which the thermal conductivity arises from vibrational excitations are known to have thermal conductivities which exhibit surprising differences from those of their insulating crystalline counterparts [2,7,14,15,26,51,50,58,61,70]. These differences are most impressively illustrated in materials which exist in both crystalline and amorphous forms; e.g., quartz and vitreous silica. The thermal conductivities of such materials at high temperatures, are not very different from one another. As the temperature is lowered, however, crystalline forms exhibit an increase of the thermal conductivity, arising from increases in the vibrational mean free path and diffusivity of vibrational pulses. On the other hand, amorphous forms, for the same temperature decrease, exhibit a decrease of the thermal conductivity arising from the decrease in the specific heat of vibrational modes. As the temperature is further decreased the thermal conductivity of crystalline forms attains a maximum below which a $T^3$ dependence, arising from the vibrational specific heat, is observed to $T = 0K$. During the same temperature decrease amorphous forms, aside from a small plateau region of constant thermal conductivity, exhibit a steady decrease in thermal conductivity and maintain thermal conductivity values which generally are much less than those of their corresponding crystalline forms. The above described regions of difference in the thermal conductivities of crystalline and amorphous materials of similar
chemical composition are also, in general, observed between crystalline and amorphous materials of different chemical composition and are generally found to occur in such samples at temperatures less than 100K.

Though there is a great difference between the thermal conductivity of crystalline and amorphous insulating solids, the thermal conductivities of amorphous insulating solids are found quantitatively as well as qualitatively to be very similar to one another. In general, three regions of temperature behavior are observed in amorphous insulating solids. These are: (1) for $T \leq 1$ K the thermal conductivity exhibits a $T^\beta$ power law behavior with $1 \leq \beta \leq 2$, (2) for $1K \leq T \leq 10K$ a plateau region is observed in which the thermal conductivity is relatively independent of temperature, (3) for $10K \leq T \leq 100K$ the thermal conductivity again exhibits a monotonic increase with increasing $T$. These three regions have been observed experimentally for example in References [7,14,15,26,51,61,70]. As these three features are present in most amorphous insulating solids, exhibiting the same order of magnitude of the thermal conductivity, a comprehensive theoretical treatment of the thermal conductivity must display the general properties discussed above for quite general amorphous geometries and atomic interactions. Below we shall present computer simulation results for the thermal conductivities of a general amorphous insulator which satisfies these conditions.

A number of theories have been put forth to explain, with greatly varying degrees of success, the thermodynamic properties of amorphous insulating solids. (For a good review of these various theories see Refs. [2,7,14,26,50,51,58].) The most successful of these theories in terms of the ability to explain the greatest number of experimental properties, however, is that which treats the scattering of vibrational waves in amorphous systems as arising from two sources. In this
theory, the first source of scattering is the scattering of the vibrational waves in the system from the randomness of the amorphous network of atoms itself. A second source of scattering arises from the fact that the amorphous network of atoms in the amorphous solid represents a metastable equilibrium state of the system and the system can have many different metastable equilibrium states. The network of atoms can hence undergo transitions between various metastable amorphous networks geometries and in the process of changing between different metastable geometries the vibrational waves of the system scatter from the transforming network geometry. This second source is generally described phenomenologically in terms of what is known as the two level states theory [2,50]. The above described theory, which combines a study of the propagation of vibrational waves in an amorphous network with the two level states theory treatment of the scattering arising from transitions between metastable states of the atomic network, offers at least a qualitative explanation of most phenomena observed in amorphous solids and will offer a basis of our discussions of the thermal conductivity of amorphous solids.

Both the determination of the propagation of vibrational waves in amorphous systems and the scattering of vibrational waves which takes place as the amorphous network of atoms transforms between metastable states are very difficult to tread exactly [2,7,50,51,58]. In particular, the two level states theory [2,50] remains an essentially phenomenological theory and until recently [58] the dynamical theory of vibrational waves on a given metastable network geometry relied on only rather crude approximations. While the two level states treatment is well established as a phenomenologically valuable description of the low temperature/low frequency properties of amorphous solids [7,51], it is only with the
development of high speed computers that an essentially exact treatment for the vibrational excitations on a realistic model network of a metastable realization of an amorphous system of atoms has been possible [58].

The recent computer simulation work on vibrational excitations and the thermal conductivity of amorphous insulating materials has been done by Sheng and Zhou [58]. In this work Sheng and Zhou considered a scalar wave treatment of the vibrational properties of a system of atoms on an infinite percolating cluster. The percolating cluster geometry then simulated the network geometry of an amorphous material, and the scalar wave theory of atomic displacements was used to simplify the numerical solution of the vibrational waves in the system. This system was modeled by an array of such atoms generated in the memory of a computer, and Newton's equations of motion were used to numerically compute the diffusion constant of a vibrational pulse centered in frequency space about a vibrational frequency, $\omega$, for a scalar wave model of atomic displacement in the percolating cluster. Recursive methods [16,42,43] were then used to obtain the density of states of the percolating scalar wave system. From these two scalar wave results, taken in combination with the two level states theory [2,14,50,58] treatment of scattering accompanied by changes in the metastable state geometry of the amorphous network, Sheng and Zhou computed the thermal conductivity of the amorphous system.

The scalar wave results of Sheng and Zhou for the thermal conductivity of amorphous networks are found to exhibit correctly the three temperature regions and behaviors discussed above. In addition, for appropriate choices of model parameters, good agreement with experimental results on a wide variety of experimental systems was obtained, and results are found to be only moderately
sensitive to the overall choice of model parameters. This moderate sensitivity of the thermal conductivity on system parameters is one of the characteristics we expect from a successful theory of amorphous materials [7,51]. One very important success of the Sheng and Zhou theory is, as we shall discuss below, its identification of the origin of the so-called plateau region in the temperature dependence of the thermal conductivity.

While the scalar wave results of Sheng and Zhou can be compared favorably with results on experimental systems, they do not however correctly take into account the fully three-dimensional nature of atomic displacements in amorphous systems. This is an important point as recent work indicates that significant differences can arise between the physical properties exhibited in a full vector field treatment and those displayed in scalar wave approximations of vector field theories [17,60]. In particular, recent work on photonic systems indicates that in photonic systems results obtained in the scalar wave approximation can exhibit important differences with corresponding results obtained using a fully vector treatment of the electromagnetic fields [17,60]. Scalar wave approximation solutions to the photonic systems more readily exhibit photonic band gaps in periodic systems and more readily displays localized states than do fully vector treatments of the electromagnetic fields. We expect similar differences in the band structures and localization properties of vibrational systems.

In light of the differences that are encountered between the scalar wave approximation and fully vector treatments in photonic systems, we present below an extension of the treatment of Sheng and Zhou to handle vibrational systems in which the atoms of the amorphous system are allowed fully three-dimensional (vector) vibrational displacements rather than the one-dimensional displacements...
found in the scalar waves theory. We shall find that many of the properties of the scalar wave theory are retained in the full vector wave treatment for the thermal conductivity of amorphous insulating solids.

II.2. The Model for Thermal Conductivity Calculation

We base our calculations for the thermal conductivity $K(T)$ of an amorphous solid on the expression:

$$K(T) = \int_0^\infty \nu(\omega)C(\omega)D(\omega)d\omega$$  \hspace{1cm} (II.1)

where $\nu(\omega)$ is the phonon density of states in frequency, the specific heat at temperature $T$ of the vibration modes of frequency $\omega$ is equal to

$$C(\omega) = k_B \left( \frac{\hbar \omega}{k_B T} \right)^2 \frac{\exp((\hbar \omega)/(k_B T))}{\left[\exp((\hbar \omega)/(k_B T)) - 1\right]^2}$$  \hspace{1cm} (II.2)

and $D(\omega)$ is the diffusion constant of a phonon of frequency $\omega$. Equation (II.1) does not make a distinction between the diffusivity of different types of modes of frequency $\omega$, but rather treats all excitations of frequency $\omega$ the same. This is not unreasonable as statistically the properties of amorphous materials are isotropic. In addition $D(\omega)$ as computed in our computer simulation studies below is found to be independent of the initial configurations of the pulses used to compute $D(\omega)$.

From the simple form of Eq. (II.1) it has been argued that the temperature dependence of $K(T)$ can be explained qualitatively in terms of the frequency dependence of $D(\omega)$ or, equivalently, the frequency dependence of the phonon mean free path $l(\omega)$ which is proportional to $D(\omega)$ [7,14,51]. Specifically, three
regions of frequency dependence are proposed. These are: (1) at low frequencies \( D(\omega) \) is very large and is due to the scattering of phonons with two-level states representing the transition of the amorphous crystal structure between its various metastable states, (2) as the frequency is increased \( D(\omega) \) decreases and phonon scattering becomes dominated by Rayleigh scattering of phonons from the amorphous geometry \([19,21]\), (3) at frequencies above the region dominated by Rayleigh scattering \( D(\omega) \) is small and relatively frequency independent up to the maximum vibrational frequency in the system. The amorphous solid, hence, behaves like a low pass filter for phonon transport \([14]\). These three regions were observed in the computer simulation of Sheng and Zhou \([58]\), and are again found in the results for the fully three-dimensional system we present below.

To compute \( K(T) \) we need to determine \( \nu(\omega) \) and \( D(\omega) \) for a specific realization of an amorphous structure. This has recently been done by Sheng and Zhou \([58]\) for a scalar displacement field on a cubic percolating network. In our simulation studies presented below, however, we considered a more realistic model of an amorphous network, allowing fully three dimensional motion of the atoms in the system. We have chosen for these studies the simplest such generalization of the system treat by Sheng and Zhou \([58]\). This is composed of atoms taken to be on an infinite percolating cluster of a fcc lattice and interacting by nearest neighbor Lennard-Jones pair potentials. We choose the Lennard-Jones pair potential as it is one of the most commonly used pair potential in theoretical treatments of atomic systems. The choice of nearest neighbor pair potentials to model the atomic interactions in our amorphous structures, however, precludes a treatment based on the geometry of the simple cubic lattice as the simple cubic lattice with nearest neighbor pair potential interaction is mechanically unstable.
The Hamiltonian of the system we study is then

\[ H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_i \sum_{\delta} u(|r_{i+\delta} - r_i|) \]  

where \( i \) runs over the atoms, \( \delta \) is such that \( i+\delta \) sums over the nearest neighbors of the \( i^{th} \) atom, \( \{r_i\} \) are the atomic positions, \( \{p_i\} \) are the atomic momentums and

\[ u(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \]

is the (12-6) Lennard-Jones pair potential. We further assume that the system has no external stress applied to it so that the fcc lattice constant \( a_0 = 2^{\frac{1}{3}} \sigma \). From this system we remove at random a fraction \( 1 - p \) of the atoms so that \( p \gg 0.119 \) is the fractional concentration of the remaining atoms on the fcc lattice. Once this is done we then further remove all atoms in finite clusters, retaining only the atoms bound in the infinite percolating cluster. The remaining atoms are at the sites they occupied in the original fcc lattice, i.e., there is no relaxation of the percolating cluster.

For the computation of \( \nu(\omega) \) the dynamics of the atoms on the above described percolating cluster are obtained in the harmonic approximation. The dynamical matrix of the cluster is computed using the pair potential in Eq. (II.4), and \( \nu(\omega) \) for the cluster is obtained from the dynamical matrix using recursive methods [16]. On the other hand, for the computation of \( D(\omega) \) the dynamics of atoms in the above described percolating cluster are obtained using the full anharmonic Hamiltonian in Eq. (II.3). The difference between \( D(\omega) \) computed using the harmonic approximation or the full anharmonic Hamiltonian is slight.
so that we have used the more complete, anharmonic, treatment in the results presented below. In the following, we shall first discuss the recursive method computation of \( \nu(\omega) \). Following this we give a discussion of the computation of \( D(\omega) \).

II.3. Density of States Calculation

Our density of states calculations are based on the work by Haydock et al [16], involving recursive methods, and the works by Nex [42,43], involving recursive termination schemes. The density of vibrational modes in \( \omega \) of our random network, \( \nu(\omega) \) (where

\[
\nu(\omega) d\omega = n(\omega^2) d\omega^2,
\]

and \( n(\omega^2) \) is the density of modes in \( \omega^2 \), can be written in terms of a summation over the local density of states \( n_{i,\alpha}(\omega^2) \) at each atomic site \( i \) for the component of atomic motion along the \( \alpha \)-axis, e.g.,

\[
n(\omega^2) = \sum_{i,\alpha} n_{i,\alpha}(\omega^2)
\]

where \( \int n_{i,\alpha}(\omega^2) d\omega^2 = 1 \). Specifically, in terms of the dynamical matrix \( D \) of the vibrational system

\[
n_{i,\alpha}(\omega^2) = -\frac{1}{\pi} \text{Im} G_{ii,\alpha}(\omega^2)
\]

where

\[
n_{i,\alpha}(\omega^2) = -\frac{1}{\pi} \text{Im} G_{ii,\alpha}(\omega^2) = \left< i, \alpha \left| \omega^2 + i0 - D \right|^{-1} \right| i, \alpha \right>
\]
and \(|i, \alpha\) is a normalized state of motion of the \(i\)th atom along the \(\alpha\)-axis.

\(G_{i,i}^{\alpha,\alpha}(\omega^2)\) can be computed using recursive techniques. Using these techniques the dynamical matrix \(\mathcal{D}\) transforms to the tridiagonal form

\[
\mathcal{D}_{mn}^{\alpha,\alpha} = \begin{cases} 
    a_m^{i,\alpha} & n = m \\
    b_m^{i,\alpha} & n = m + 1 \\
    b_m^{i,\alpha} & n = m - 1 \\
    0 & \text{otherwise}
\end{cases}
\] (II.9)

from which \(G_{i,i}^{\alpha,\alpha}(\omega^2)\) can be expanded as a continued fraction

\[
G_{i,i}^{\alpha,\alpha}(\omega^2) = \frac{1}{\omega^2 - a_1^{i,\alpha} - |b_2^{i,\alpha}|^2 \frac{1}{\omega^2 - a_2^{i,\alpha} - |b_3^{i,\alpha}|^2 \frac{1}{\omega^2 - a_3^{i,\alpha} - |b_4^{i,\alpha}|^2 \frac{1}{\omega^2 - a_4^{i,\alpha} - \ldots}}}}
\] (II.10)

where

\[
a_n^{i,\alpha} = \langle V_n^{i,\alpha} | \mathcal{D} | V_n^{i,\alpha} \rangle , \quad (II.11a)
\]

\[
b_{n+1}^{i,\alpha} = \sqrt{\langle \tilde{V}_{n+1}^{i,\alpha} | \tilde{V}_{n+1}^{i,\alpha} \rangle} \quad (II.11b)
\]

\[
|\tilde{V}_{n+1}^{i,\alpha} \rangle = (\mathcal{D} - a_n^{i,\alpha} I) |V_n^{i,\alpha} \rangle - b_n^{i,\alpha} |V_{n-1}^{i,\alpha} \rangle \quad (II.11c)
\]

\[
|V_{n+1}^{i,\alpha} \rangle = \frac{1}{b_{n+1}^{i,\alpha}} |\tilde{V}_{n+1}^{i,\alpha} \rangle \quad (II.11d)
\]

\[
b_1^{i,\alpha} = 0 \quad (II.11e)
\]

\[
|V_0^{i,\alpha} \rangle = 0 \quad (II.11f)
\]

\[
|V_1^{i,\alpha} \rangle = |i, \alpha\rangle \quad (II.11g)
\]
In general, for the calculations presented below, we have used Eq. (II.11) to generate about 20 to 40 sets of \( \{ a^{i,\alpha}, b^{i,\alpha} \} \) for a given \( |i, \alpha \rangle \). These are then used in Eq. (II.10) along with some appropriate termination scheme to evaluate \( G_{i,i}^{\alpha,\alpha}(\omega^2) \) and subsequently \( n_{i,\alpha}(\omega^2) \) and \( n(\omega^2) \).

The termination scheme allows for the approximation of the infinite continued fraction in Eq. (II.10) by a finite continued fraction which has been ended in its last term by an appropriately chosen function of \( \omega^2 \). The chosen function of \( \omega^2 \) represents an approximation of the remainder terms dropped from the continued fraction in order to give it a finite representation. In the results presented below for \( n(\omega^2) \), we used the termination scheme introduced in Refs. [42,43]. This termination involves the development of an expression for \( n_{i,\alpha}(\omega^2) \) from its continued fraction representation and the derivative of \( \int_{\omega^2} n_{i,\alpha} d\omega^2 \) with respect to \( \omega^2 \). The realization of this method for our problem is described in Section II.7.

We have considered a cubic array of fcc lattice of 21 x 21 x 21 conventional unit cells consisting of 37,044 lattice sites, applying periodic boundary conditions at the faces of the array. With the use of a random numbers generator a fraction \( p \) of the lattice sites can be randomly chosen to be occupied by atoms. Then all isolated clusters are removed and the largest percolation cluster is chosen for study. A pure, \( p = 1 \), fcc atomic system then consists of 37,044 atoms on the lattice, and for \( 0 \leq p \leq 1 \) there are a little less than 37,044\( p \) atoms on the lattice (isolated atomic clusters are removed). In computing \( n(\omega^2) \) we have determined \( n(\omega^2) \) using 1000 and 6000 different \( |i, \alpha \rangle \) chosen at random. Little difference was found between \( n(\omega^2) \) computed using 1000 and \( n(\omega^2) \) computed using 6000. In Figure 1 we present continued fraction results for \( n(\omega^2) \) versus \( \omega^2 \) for the pure \( p = 1 \) system. These results agree well with \( n(\omega^2) \) computed in [68].
Figure 1. The Density of States \( n(\omega^2) \) Versus \( \omega^2 \) for a Pure System \((p = 1)\), Composed of \( N \) Atoms.

In Figure 2 results are shown for \( n(\omega^2) \) on the infinite percolation cluster versus \( \omega^2 \) for \( p = 0.9, p = 0.8, \) and \( p = 0.7 \). The density of states in these plots is observed to smoothly shift for decreasing \( p \) to forms which concentrate modes in regions of low frequency. This softening of the network is to be expected but cannot be used by itself to account for the transitions observed between the three temperature regions in \( K(T) \) for \( T \leq 100K \).

As a check on the results in Figure 2 we compare in Figure 3 some of these results to results for \( n(\omega^2) \) obtained by directly counting of eigenvalues of the dynamical matrix computed for a reduced array of 864 sites. The agreement
between $n(\omega^2)$ computed in these two ways is good.

II.4. Diffusion Coefficient Calculation

The phonon diffusion coefficient $D(\omega)$ for phonons of frequency $\omega$ is composed from two different components [14,58]. One component arises from the propagation of the $\omega$ frequency vibration through the random network of fixed geometry. In this propagation the atoms on the network are only allowed to exhibit small vibrations about the fixed positions they occupy in the absence of vibrational excitations. A second component arises from the scattering of the $\omega$
frequency vibration from changes in the geometry of the random network as the random network transforms between its various metastable states of equilibrium. During these transformations between metastable states of the network, the fixed positions the atoms of the network occupy in the absence of vibrational excitations are changed to reflect a new equilibrium configuration of the atoms of the network.

The phonon diffusion coefficient $D(\omega)$ is proportional to the total mean free
path \( l(\omega) \) for phonon scattering in the system. In terms of the phonon scattering processes discussed above we shall assume that [14,58]

\[
\frac{1}{l(\omega)} = \frac{1}{l_N(\omega)} + \frac{1}{l_{TL}(\omega)} 
\]  

(II.12)

where \( l_N(\omega) \) is the mean free path for phonon scattering for a fixed network geometry and \( l_{TL}(\omega) \) is the mean free path for phonon scattering accompanying a change in the network geometry between metastable states. The assumed relations between \( l(\omega) \) and the two processes given by \( l_N(\omega) \) and \( l_{TL}(\omega) \) which contribute to form \( l(\omega) \) is commonly observed for multiple channel decay processes and assumes the additivity of the transition probabilities of the two types of scattering events. Using the fact that the diffusion coefficient, \( D_N(\omega) \), for processes only involving scattering from a fixed network is proportional to \( l_N(\omega) \) and that the diffusion coefficient, \( D_{TL}(\omega) \), for processes only involving scattering accompanying a change in network geometry between metastable states is proportional to \( l_{TL}(\omega) \), we find from Eq. (II.12) that

\[
\frac{1}{D(\omega)} = \frac{1}{D_N(\omega)} + \frac{1}{D_{TL}(\omega)} 
\]  

(II.13)

In the calculations present below we shall assume that Eq. (II.13) holds between the two types of diffusion coefficients defined above.

The processes contributing to \( D_{TL}(\omega) \) are difficult to treat as they involve changes between metastable states of the network geometry. These processes are commonly treated in the context of the two-level state theory proposed independently by Anderson, Halperin and Varma [2] and by Philips [50]. This is a phenomenological treatment which uses the general form
\[
\frac{1}{\tau_{\text{TL}}(\omega)} = A \frac{\hbar \omega}{k_B} \tanh \left( \frac{\hbar \omega}{2k_B T} \right) + \frac{A}{2} \frac{1}{\frac{k_B}{\hbar \omega} + \frac{1}{BT^3}}.
\] (II.14)

for fitting parameters \(A\) and \(B\) to give the low temperature behavior of \(\tau_{\text{TL}}(\omega)\). (Eq. (II.14) was taken from the Ref. [14] and differs from that used by Sheng and Zhou [58]) The diffusion coefficient \(D_{\text{TL}}(\omega) = \frac{2}{3} \tau_{\text{TL}}(\omega)\) where \(\bar{v}\), the average phonon velocity, gives the new fitting parameters \(\bar{v}A\) and \(B\). \(D_{\text{TL}}(\omega)\) computed from (II.14) dominates the low frequency behavior of \(D(\omega)\) in the region in which \(D_N(\omega) \propto \omega^{-4}\) arises mainly from Rayleigh scattering but does contribute significantly to \(D(\omega)\) at higher frequencies.

In the context of our percolation model of a random network, \(D_N(\omega)\) can be computed using standard molecular dynamics routines which integrate the classical mechanical equations of motion. This is done for the atoms interacting by nearest neighbor pair potentials, in a full anharmonic treatment of the motion of the atoms in the system. We treat the system using classical mechanics because the classical equations of motion are easily integrated and are known to reproduce the quantum dispersion relation of vibrational systems correctly such that many of the thermal properties of these systems are obtained by using classical mechanical results combined with the assumption of Bose statistics. In the following we shall assume that the mixture of a classical mechanical \(D_N(\omega)\) with the assumption of Bose statistics is valid in the application of Eq. (II.1) for the computation of \(K(T)\).

In computing \(D_N(\omega)\) we treat only atoms on the infinite percolating cluster. In the context of the computer simulation this is the largest remaining cluster after all isolated small clusters of atoms are removed from the system. We assume that initially no vibrational excitations are present on the percolating cluster. Using the classical equations of motion we then study the motion of the atoms in the
system when, to a single atom at the center of the percolating cluster, we apply a time-dependent force of the form

$$F(t) = \begin{cases} F_0 \sin(\omega t) \exp\left(-\frac{(\gamma \omega t)^2}{2}\right), & -t_0 \leq t \leq t_0 \\ 0, & \text{otherwise} \end{cases}$$ \hspace{1cm} (II.15)$$

where $F_0$ is a randomly chosen force vector, the coefficient $\gamma$ deals with the spectral width of the force from Eq. (II.15) so that $F'(\omega) \propto \exp\left(-\frac{(\omega-\omega_c)^2}{2\gamma^2}\right)$, and the value of $t_0$ has been chosen such that $|\gamma \omega t_0|^2 \geq 3.8$. The simulation begins at $t = -t_0$ and proceeds until the disturbances produced by $F(t)$ reaches the edge of the finite array of atoms in the computer memory.

The force in Eq. (II.15) drives the system in a band of frequencies centered about $\omega$. The amplitude distribution of the driving force as a function of frequency has a half width at half maximum of $\Delta \omega \approx 2\gamma \omega$. Consequently, the pulse generated by Eq. (II.15) represents a sampling of the frequency response of the system averaged over the frequencies between $\omega - \Delta \omega$ and $\omega + \Delta \omega$. By studying the diffusion of the vibrational excitation created by this force pulse, we arrive at an approximation for $D_N(\omega)$ which becomes increasingly more accurate as $\Delta \omega$ decreases. The choice of $\Delta \omega$ used in the numerical integration must be as small as possible within the simulation constraints of creating a spatially narrow vibrational pulse to travel over the finite sized network stored in the computer memory. For the systems studied with our simulation $\Delta \omega \approx 0.07 \omega$.

The diffusion coefficient, $D_N(\omega)$, is computed by creating a vibrational pulse from Eq. (II.15) and studying the time dependence of the vibrational pulse created by the force defined in Eq. (II.15). Specifically, we compute
\[ \langle R^2 \rangle = \frac{\sum_i u_i R_i^2}{\sum_i u_i} \]  
(II.16)

where \( R_i \) is the equilibrium position vector of the \( i \)th atom in the percolating cluster measured relative to the equilibrium position of the atom driven by the force defined in Eq. (II.15), \( i \) runs over all of the atoms of the percolating cluster and

\[ u_i = \frac{p_i^2}{2m} + \frac{1}{2} \sum_\delta u(|r_{i+\delta} - r_i|) \]  
(II.17)

where \( r_i \) is the position of the \( i \)th atom in the presence of the vibrational pulse and the sum on \( \delta \) runs over the nearest neighbors of the \( i \)th atom on the percolating cluster. After the initial transients have died down, the long time behavior of is described by

\[ \langle R^2 \rangle = 6D_N(\omega)t + \text{const} \]  
(II.18)

so that the diffusion coefficient is obtained from the slope of \( \langle R^2 \rangle \) computed as a function of time. The choice of \( u_i \) in Eq. (II.16) and (II.17) which is roughly the vibrational energy of the \( i \)th atom, is a logical choice of a physical quantity to use in the computation of \( \langle R^2 \rangle \) and \( D_N(\omega) \). It, however, is not the only choice and for example various linear combinations of \( \frac{p_i^2}{2m} \) and \( \frac{1}{2} \sum_\delta u(|r_{i+\delta} - r_i|) \) can be used to evaluate \( \langle R^2 \rangle \). We have found that \( u_i \) in Eq. (II.17) avoids short period oscillatory behavior in \( \langle R^2 \rangle \) which is present, after the initial transitions in time have disappeared, in other forms for \( u_i \). For forms of \( u_i \) which exhibit short period oscillations in \( \langle R^2 \rangle \), short time interval averages of \( \langle R^2 \rangle \) need to be performed in
order to extract $D_N(\omega)$. The $D_N(\omega)$ computed from $u_i$ in Eq. (II.17) or its other various forms do not, however, differ substantially from one another (see Ref. [20]).

In Figure 4 we present results for the diffusion coefficient, $D_N(\omega)$, as a function of frequency for $p = 0.55$, $p = 0.7$ and $p = 0.8$. The solid lines in this figure represent $D_N(\omega)$ computed as described above but the dashed lines represent interpolation for $D_N(\omega)$ which we discuss below. These results were obtained for percolating clusters created from an fcc region of $37 \times 37 \times 37$ conventional unit cells (202,612 atoms sites) subject to periodic boundary conditions. In computing
$D_N(\omega)$ the force function given in Eq. (II.15) was set up with parameters such that $D_N(\omega)$ at frequency $\omega$ is actually $D_N(\omega)$ averaged over the frequency region $\omega \pm 0.07\omega$.

At low frequencies ($\omega/\omega_{\text{max}} \lesssim 0.2$), due to the onset of Rayleigh scattering, the diffusion coefficient becomes large as $\omega$ decreases. Consequently, $D_N(\omega)$ becomes increasingly more difficult to compute using the numerical procedure discussed above as the vibrational pulse begins to hit the boundaries of array of 202,612 sites before the system settles down to the behavior, indicated in Eq. (II.18). It is well known, however, that at low frequencies $D_N(\omega)$ is dominated by Rayleigh scattering (see for example [19] Sect. 9.7, 9.8 , [21] and references there) so that $D_N(\omega) \xrightarrow{\omega \to 0} C_d \omega^{-4}$. This fact can be used to estimate the low frequency behavior of $D_N(\omega)$ in the region of $\omega$ in which the simulation fails. Specifically, in Figure 4 at low frequency we have approximated $D_N(\omega) = C_d \omega^{-4}$ (dotted lines at low frequency) where $C_d$ is chosen to match the simulation results for $D_N(\omega)$ (solid lines) at their lowest frequency. We shall discuss this approximation in our conclusions below, where we find that the thermal conductivity results are rather insensitive to the value of $C_d$ chosen for the $D_N(\omega) = C_d \omega^{-4}$ limiting form.

At the upper frequency limit of $D_N(\omega)$, we again use an interpolation scheme to set $D_N(\omega)$ to zero at the upper frequency band edge of our vibrational system (see for example Ref. [20] ). In this case we use a linear interpolation from the upper edge of the simulation computed $D_N(\omega)$ (solid lines) to zero at $\omega = 0.96\omega_{\text{max}}$ for $p = 0.7$ and $\omega = 0.97\omega_{\text{max}}$ for $p = 0.8$, where $\omega_{\text{max}}$ is the upper band edge of the $p = 0.1$ system. The $D_N(\omega)$ values in the small region $0.88 \leq \omega/\omega_{\text{max}} \leq 1$ are difficult to compute with a high degree of accuracy using our simulation but do not contribute significantly to the thermal conductivity.
results computed below.

For all concentrations used in obtaining the results of Figure 4 we see similar behaviors for $D_N(\omega)$ as a function of $\omega$ to those postulated by Graebner et al. [14] on quite general ground as necessary for Eq. (II.1) to correctly give the qualitative behavior of $K(T)$ on $T$ obtained experimentally. These three regions were more recently exhibited in the scalar wave simulation of Sheng and Zhou, and our three-dimensional results are in general qualitative and order of magnitude quantitative agreement with the results of Sheng and Zhou. Specifically, as in Ref. [58] $D_N(\omega)$ is found to decrease in magnitude with decreasing $p$. The region in which Rayleigh scattering becomes important is, also, seen to occur at lower $\omega$ for decreasing $p$.

We shall now turn to a discussion of the computation of $K(T)$ using the results of Sections II.2 through section II.4. This will include a discussion of the sensitivity of the results for $K(T)$ on the approximations involved in computing $D_N$.

II.5. Thermal Conductivity Calculation

The model presented above for a percolating cluster of atoms interacting by nearest neighbor Lennard-Jones pair potentials is a model for an amorphous solid. While it does not directly correspond to an amorphous material which has been studied experimentally, we know that all experimentally studied amorphous materials exhibit very similar thermal conductivities to one another, all of which include the three regions of temperature dependence discussed in Section II.1. With these facts in mind we hope, then that for a wide range of parameters our model will exhibit similar thermal conductivities, including the three tempera-
tured dependencies discussed in Section II.1, to those seen in general amorphous materials.

In order to compute the thermal conductivity of our model we need to use the results for the density of states from Eq. (II.6) in Section II.3, the results from Eqs. (II.13), (II.14) and (II.18) in Section II.4 for the diffusion coefficient, and the specific heat from Eq. (II.2) to evaluate Eq. (II.1) for the thermal conductivity as a function of $T$. The resulting integral for the thermal conductivity depends on the fcc lattice constant $a_0$, $\omega_{\text{max}}$, the average phonon velocity $\bar{v}$, $A$ and $B$ as parameters which need to be assigned for a comparison with experiments. A range of experimental values for these quantities can be roughly extracted from experimental results obtained by Graebner et al (see Table 1 of Graebner et al [14]) for a large number of different amorphous materials, and we shall base the thermal conductivity results presented below on values for $a_0$, $\omega_{\text{max}}$, $\bar{v}$, $A$ and $B$ from these experiments. In general, we find below that the behavior of $K(T)$ is only moderately sensitive to the spectrum of values for $a_0$, $\omega_{\text{max}}$, $\bar{v}$, $A$ and $B$ obtained from the data of Graebner et al [14].

In computing the thermal conductivity, values for $\bar{v}$, $A$ and $B$ are listed in Table 1 of the work by Graebner et al [14], and we have taken these over directly in obtaining the result for $K(T)$ presented below. To obtain values of $\omega_{\text{max}}$ we have made the approximation $\hbar\omega_{\text{max}} = k_B \Theta_D$, where $\Theta_D$ is the Debye temperature and have used the values of $\Theta_D$ listed in Table 1 of Ref. [14]. A values of the lattice constant $a_0$ can be obtained from

$$a_0 = a_1 p^b$$  \hspace{1cm} (II.19)

where $p$ is the percolation concentration and
where \( g \) is the mass density (taken from Table 1 of Ref. [14]), \( m_{\text{unit}} \) is the mass of the molecular unit which is repeated on the amorphous network, and \( q_{\text{unit}} \) is the number of atoms in the molecular unit. Equations (II.19) and (II.20) have been chosen so that the number of vibrational modes per volume is the same in our model as in the experimental material we compare with.

**Table 1**

Parameters We Used for the Thermal Conductivity Calculation

<table>
<thead>
<tr>
<th>Material</th>
<th>( g )</th>
<th>( \bar{v} )</th>
<th>( \Theta_D )</th>
<th>( A )</th>
<th>( B )</th>
<th>( m_{\text{unit}} )</th>
<th>( q_{\text{unit}} )</th>
<th>( a_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a-\text{SiO}_2 )</td>
<td>2.2</td>
<td>4.1</td>
<td>300</td>
<td>360</td>
<td>3.0</td>
<td>60.08</td>
<td>3</td>
<td>2.78</td>
</tr>
<tr>
<td>( a-\text{Se} )</td>
<td>4.3</td>
<td>1.19</td>
<td>113</td>
<td>880</td>
<td>20.0</td>
<td>78.96</td>
<td>1</td>
<td>3.51</td>
</tr>
<tr>
<td>PMMA</td>
<td>1.2</td>
<td>1.79</td>
<td>150</td>
<td>1000</td>
<td>0.3</td>
<td>100.12</td>
<td>15</td>
<td>2.36</td>
</tr>
</tbody>
</table>

In the Table 1 we present parameters we have extracted from the Graebner et al data for \( a-\text{Se} \), \( a-\text{SiO}_2 \) and PMMA, and which we use in our calculation of \( K(T) \) below. We have chosen these materials to base our calculations on as they yield the most diverse set of values for the parameters set in Table 1.

In Figures 5 and 6 we present \( K(T) \) versus \( T \) computed in the above described manner for \( p = 0.7 \) and \( p = 0.8 \), respectively. The results for \( p = 0.7 \) and \( p = 0.8 \) are very similar to one another, and all exhibit the three regions of temperature dependence observed in the thermal conductivity of amorphous...
materials for $T \leq 100K$. While there is a qualitative agreement between the thermal conductivities in Figure 5 and Figure 6, computed from parameters based on those for $a$–Se, $a$–SiO$_2$ and PMMA found in Ref. [14], and the experimental data for these materials presented in Figure 2 of Ref. [14], we do not expect nor do we find quantitative agreement between our Figures 5, 6 results and the Graebner et al [14] results in their Figure 2. This is due to the fact that our Lennard–Jones percolating model does not reflect the structure of $a$–Se, $a$–SiO$_2$ and PMMA. The success of our model is in the fact that for reasonably chosen values of the parameters in our model we observe $K(T)$ which is consistent with $K(T)$ behavior.
observed in data obtained experimentally from amorphous materials. One problem with our results, however, is a tendency of the model to give too large values of $K(T)$ at low temperatures. This problem arises from the large values of our density of states $\nu(\omega)$ at lower frequencies, and may be an artifact arising from our use of a percolating cluster to model an amorphous network.

All of curves presented in Figures 5 and 6 display the three regions of thermal conductivity, observed in amorphous insulating materials. These three regions, as we discuss below, are founded in our full vector treatment to arise from the same general factors which give rise to them in the scalar wave treatment.
and are temperature regions generally observed in the thermal conductivity of amorphous insulating materials.

Specifically, at low temperature \((T \lesssim 1\text{K})\) in which the diffusivity is dominated by two level scattering, we find \(K(T) \propto T^\beta\), where at low frequencies \(\nu(\omega) \propto \omega^\alpha\). Our results for \(p = 0.8\) exhibit Debye behavior for \(\omega/\omega_{\text{max}} \lesssim 0.2\) and give \(\beta = 2\) but our \(p = 0.7\) results, which only exhibit Debye behavior for \(\omega/\omega_{\text{max}} \lesssim 0.05\), give \(1 < \beta < 2\). These types of power law behaviors compare favorably with experiment and with the results of the scalar wave theory [58]. The scalar wave results of Sheng and Zhou, however, are based on models which exhibit a stiffer vibrational spectra and give only \(\beta = 2\).

All of the results in Figures 5, 6 exhibit a plateau region between \(1\text{K} \lesssim T \lesssim 10\text{K}\). This region, as in the scalar wave theory of Sheng and Zhou, arises from the low pass filter characteristics of the amorphous vibration network. In this regards the \(C_d\omega^{-4}\) contribution to \(D_N(\omega)\) from Rayleigh scattering is important in determining the low temperature limit of the plateau region. This can be seen from Figure 7 in which we plot the thermal conductivity versus temperature for \(p = 0.8\) for the parameters extracted for PMMA. Results are shown for \(C_d, 2C_d, 4C_d\), where \(C_d\) is the Rayleigh scattering fitting coefficient used in Figure 6 for PMMA. Results are also shown for the \(C_d \to \infty\) limit of the Rayleigh scattering, \(C_d\omega^{-4}\), term in \(D_N(\omega)\). This removes the Rayleigh scattering from the system. We see in general, for parameters \(C_d, 2C_d, 4C_d\) the character of the thermal conductivity is little changed from the \(C_d\omega^{-4}\) fit. In the extreme limit that Rayleigh scattering is ignored a small plateau region is still observed but the thermal conductivity determined in this case is too large by an order of magnitude when compared to experimental results. In this last limit the plateau region is,
Figure 7. Test for the Thermal Conductivity, Calculated for Table 1 PMMA Parameters for $p = 0.8$ With $C_d (1)$, $2C_d (2)$, $4C_d (3)$, and Without Rayleigh Scattering at Low Frequencies (4).

also, observed to begin at too large a value of $T$ compared to those observed in experimental systems.

Above the plateau region, for $T \gtrsim 20K$, all curves in Figures 5, 6, 7 are observed to display $K(T)$ which increase monotonically with increasing $T$. This behavior follows primarily from $C(\omega)$ in Eq. (II.2) and its increase with increasing $T$. 

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II.6. Conclusion

We have computed the thermal conductivity of a model composed of a fcc percolating cluster of atoms. Unlike previous treatments we have allowed the atoms in the system to undergo full three dimensional motion. We find upon comparison with the scalar wave treatment that:

1. Both models exhibit diffusion coefficients which decrease in magnitude with decreasing atomic concentration $p$. The Rayleigh scattering dominates $D_N(\omega)$ at lower frequencies as $p$ is decreased. At lowest frequencies the total diffusivity is determined by two level states scattering. As the frequency is increased a region is observed in which the total diffusivity is dominated by Rayleigh scattering and at the largest frequencies general scattering from the amorphous network is dominant.

2. The vector treatment exhibits a density of states which differs considerably from the scalar wave model and accounts for the larger thermal conductivity values observed in our vector treatment. Our results, unlike the Sheng and Zhou results, exhibit a density of states which can depart (except for a very small neighborhood of $\omega = 0$) from a quadratic variation with $\omega$ at very low frequencies.

3. Both models exhibit the three regions of different temperature dependent behavior observed for $T \leq 100K$. In both models the plateau region and its lower temperature limit are determined by the Rayleigh scattering from the amorphous network. The exponent $\beta$ in our model offers $1 \leq \beta \leq 2$ which is more realistic than $\beta = 2$ observed in the scalar wave treatment.
II.7. Termination of the Continuous Fraction Expansion

In terminating our continued fraction we have used the termination scheme described in Eqs. (3.6) through (3.8) of Ref. [43]. In our termination scheme, however, we have replaced Eq. (3.8c) by:

\[
\frac{\partial w_i}{\partial a_{n-1}} = \frac{\left\{ q_{n-1}p_{n-2} - p'_n q_{n-2} + w_i (p'_n p'_n - p''_n p_{n-1}) \right\}}{/ p'_n} \bigg|_{E=E_i} \tag{II.21}
\]

This termination was used in the routine we received from Prof. Haydock.

This termination scheme works well in computing the general frequency dependence of \(n(\omega)\). At the very lowest frequencies (i.e. \(\omega/\omega_{\text{max}} \lesssim 0.025\), where \(\omega_{\text{max}}\) is the maximum frequency in the pure fcc system), however, \(n(\omega)\) fails to go to zero at \(\omega = 0\), but begins to exhibit a bending which would eventually take it into the negative frequency region. To correct for this we have fitted out data for \(n(\omega)\) below \(\omega/\omega_{\text{max}} \approx 0.025\) with a Debye form to give the correct \(\omega \to 0\) limiting behavior.
CHAPTER III
LOCALIZATION OF LIGHT IN OPTICAL SYSTEMS

III.1. Introduction

The Anderson localization of classical mechanical or classical electromagnetic waves in a random medium has been of great interest in the last decade [11,12,18,23,48,38,57,59,71]. As with electron systems, classical excitations in a random medium can be localized by phase coherent scattering from the randomness of the medium. In particular, these systems are always localized in one- and two-dimensional random media, no matter how weak is the scattering arising from the randomness. In three-dimensional random media, however, the mode frequencies at which excitations become localized depends on the strength of the scattering arising from the disorder. While both electron and classical wave systems exhibit the effects of Anderson localization in the transport coefficients related to these excitations, classical wave systems offer the opportunity for a more direct observation of the spatial distribution of the wavefunctions of the localized excitation modes than are currently possible for electron systems. Specifically, the field intensity and energy distribution in acoustic and optical systems can often be measured directly and these distributions are related to the localization properties of the mode wavefunctions. Even so the number of different experiments on classical waves that have directly displayed the distribution in space of the localized modes is small.

The nature of the modes in acoustical and optical systems can be directly
observed by studying the field or energy density distributions of these modes. In particular, a number of studies of such field distributions have been made in one- and two-dimensional optical systems [12, 18, 48, 71]. In random layered systems the localization in space of the wave function of electromagnetic modes can be observed by measuring the field intensity in the system for waves incident to the slabs forming a semi-infinite layered medium. Similarly, in two-dimensional random systems formed as an array of parallel axes cylinders, the localized electromagnetic modes emitted by a linear antenna parallel to the cylinder axes can again be observed by measuring the field intensity in a plane perpendicular to the axes.

Our primary concern in this dissertation is with a rather novel recent theoretical proposal by De Raedt, et al. [52], for a method to measure the spatial distribution of localized classical wave modes. De Raedt, et al. [52], considered an infinite random array of parallel axis cylinders, the array is cut along a plane perpendicular to the axes of the cylinders in the array, and the region above the cut is replaced by vacuum. A finite beam of light is made incident, from the region of vacuum, on the random region below the cut. By studying the spreading of the beam in the random media, the transverse localization of light in the system can be observed and measured. Specifically, De Raedt, et al., used a scalar wave approximation and numerical simulation methods to study the propagation of light in the system. They found that the randomness in the systems limits the radius to which a circular beam of light incident on the system will spread as the light moves along the axes of the rods. This limiting radius, which becomes infinite in a non random array of rods, is the localization length limiting the transverse (in the plane perpendicular to the rod axes) spreading of the electromagnetic modes.
of the random system.

While the theoretical results of De Raedt, et al. [52], are of great interest as a means for measuring the localized wavefunctions of light, they are based on a scalar wave approximation for the electromagnetic fields. Such scalar wave approximations for the electromagnetic field have been shown to be ineffective in accurately treating the propagation of light in a number of recent computations on random and non random optical media. In this dissertation we show the differences which can arise between investigating transverse localization effects in the scalar wave approximation and in a full vector treatment of the electromagnetic fields. Specifically, we will show that, while the general conclusion of De Raedt, et al. [52], are correct, the transverse localization properties of random systems can exhibit interesting polarization dependent effects which are not correctly treated in the scalar wave approximation.

To show the importance of polarization on transverse localization we shall study the full vector Maxwell Equations for the propagation of light in a number of different types of disordered systems. Due to the complications that arise in the full vector treatment of light we will not, however, treat the same dielectric model that De Raedt, et al. [52], consider in the scalar wave approximation. The systems we treat, however, indicate the nature of the polarization effects which may be of interest in more complicated dielectric arrays which exhibit transverse localization of light.

We shall first present a discussion of beam spreading in the propagation of light in random one–dimensional layered systems. Two model we considered: a plane waves and a beam of finite width incident obliquely on a semi–infinite random array of dielectric slabs. The solution of the fields for this case can be
obtained as a Fourier transform involving the standard transfer matrix solutions of
this system for incident planewave modes. Transverse localization effects similar
to those found by De Raedt, et al., are observed in this system for s-polarized
light. Due to Brewster angle effects [55], the transverse localization is observed
to a lesser extent in p-polarized light and is found to be absent for certain ranges
of oblique incident angles near the Brewster's angle.

Finally, we will present some preliminary results for a fully two-dimensional
disordered system. The localization effects in 2D optical systems have been stud-
ied in many works [52,54]. These 2D results exhibit strong polarization depen-
dence, but do not exhibit Brewster's angle anomaly. These results will be obtained
using some numerical simulations recently developed by Pendry, et al. [6]

III.2. Transverse Localization Effects in Layered Systems

The system we study in this section consists of a semi-infinite array of
variable alternating layers of dielectric separated by vacuum layers which have
electromagnetic waves incident on them from the vacuum region of space (see
Figure 8).

\[
\epsilon(x) = \begin{cases} 
\epsilon, & n\alpha \leq x \leq (n + 0.25 + \delta a f_n)\alpha \\
1, & \text{otherwise}
\end{cases}
\]  

(III.1)

where \( n = 0,1,2,\ldots; \) \( a \) is the one-dimensional lattice constant, \( \delta a = 0.125 \) and
\( f_n \) is a random number uniformly distributed over the interval \(-1 \leq f_n \leq 1\). The
dielectric constant \( \epsilon = 9.0 \). The choice of the values of \( \epsilon \), wavelength \( \lambda \), and \( a \) will
be discussed below in the context of some of the numerical work. The distance
between slabs \( b \) is chosen such that \( a_{\text{slab}} + b = a \).
Figure 8. The Geometry of a Semi-Infinite Array of Dielectric Slabs.

The light incident on this system is in the $x-z$ plane from the region $x < 0$. Two cases are considered: In a first case, we treat an incident plane wave with angle of incidence $\theta_i$ measured from the positive $x$-axis in the $x-z$ plane such that

$$
E_{\text{inc}}(x, z) = E_0 \exp \left[ i \left( \frac{\omega}{c} (\cos \theta_i x + \sin \theta_i z) - \omega t \right) \right]
$$

$$
x \leq 0
$$

is the electric field of the incident electromagnetic radiation. In the second case, we treat an incident beam of electromagnetic radiation with the incident electric field given by

$$
E_{\text{inc}}(x, z) = \int_{-\omega/c}^{+\omega/c} \exp (ik_x(q)x + ik_z(q)z - \omega t)A(q)\frac{dq}{2\pi}
$$

$$
k_x(q) = \sqrt{\left( \frac{\omega}{c} \right)^2 - q^2 \cos \theta_i + q \sin \theta_i}
$$

$$
k_z(q) = \sqrt{\left( \frac{\omega}{c} \right)^2 - q^2 \sin \theta_i - q \cos \theta_i}
$$
The field given by (III.3) is a superposition of planewaves. The amplitude of a plane wave with the wavevector \((k_x(q), 0, k_z(q))\) is \(A(q)\). If the incident beam is a Gaussian beam then \(A(q)\) is given by:

\[
A_{\text{gauss}}(q) = \sqrt{\frac{2\pi}{\omega}} \exp\left(-\frac{(q\omega)^2}{4}\right)
\]  

(III.6)

where \(\omega\) is the beam's width in the point \((0,0,0)\). The formulae (III.4) and (III.5) transform parallel and perpendicular components (relatively to the direction of beam incidence) to \(x - z\) axes, and \(\theta_i\) is the value of incidence angle.

For both cases Eq. (III.2) and (III.3), we have considered both \(p\)-polarization (Magnetic field is along \(y\) axis) and \(s\)-polarization (Electric field is along \(y\) axis) cases for the incident beam. Due to the translational symmetry in the \(y - z\) plane, the polarization and \(k_y\) component of the wavevector of the electromagnetic fields are conserved as the electromagnetic radiation passes through the layered array of slabs. The conservation of \(k_z\) means that the wavevector \((k_x, 0, k_z)\) is the same for incident and transmitted waves. As we shall see below this fact allows us to express the transmission coefficient for a beam propagated through a finite array of slabs as a weighted superposition of planewave transmission coefficients.

First, we consider the case in which the incident wave on the system are plane waves. After this we treat the case in which incident finite beams of light are incident on the system. Following Ref. [69] the transmission coefficient calculation for the incident planewave, Eq. (III.2), has been done by using the transfer matrix method.
III.3. The Transfer Matrix Method

Transfer matrix approach can be applied in the case if incident wave is a planewave. The solution for a beam can be obtained as a superposition of plane waves. In this section we study a plane wave of the form (III.2) incident on the system. Because our system is invariant with respect to translation in the $z$ direction and rotation about the $x$ axis, we can write the electric field $\mathbf{E}$ inside the system in the following form:

$$\mathbf{E}(x) = \mathbf{E}(x) \exp(ik_x x) \exp(i\omega t)$$  \hspace{1cm} (III.7)

From Maxwell's equations

$$\text{rot} \mathbf{E} = -\frac{1}{c} \frac{\partial B}{\partial t}$$  \hspace{1cm} (III.8a)

$$\text{rot} \mathbf{B} = \frac{1}{c} \frac{\partial E_x}{\partial t}$$  \hspace{1cm} (III.8b)

$$\text{div} \mathbf{B} = 0$$  \hspace{1cm} (III.8c)

$$\text{div} \mathbf{E} = 0$$  \hspace{1cm} (III.8d)

we then find that $\mathbf{E}(x)$ from (III.7) has the following form:

$$\mathbf{E}(x) = \begin{cases} A_n \exp(-iq_v x) + B_n \exp(iq_v x) & \text{for } x \text{ in the vacuum} \\ C_n \exp(-iq_m x) + D_n \exp(iq_m x) & \text{for } x \text{ in the slab} \end{cases}$$  \hspace{1cm} (III.9)

In Eq. (III.9) the index $n = 0, 1, 2, \ldots$ labels the layers and

$$q_v = \frac{c}{\varepsilon} \cos(\theta)$$  \hspace{1cm} (III.10a)

$$q_m = \frac{c}{\varepsilon} \cos(\theta_m)$$  \hspace{1cm} (III.10b)

$$\theta_m = \arcsin(\sin(\theta) / \sqrt{\varepsilon})$$  \hspace{1cm} (III.10c)
Due to the one-dimensional nature of the system, we can separate the electromagnetic waves into cases of s and p polarizations. We define the s polarization as the polarization in which \( E(x) = (0, E_y, 0) \) and the p polarization as the polarization in which \( B(x) = (0, B_y, 0) \). Because of the above mentioned symmetry in the \( y-z \) plane, these polarizations do not mix with one another.

The boundary conditions on the slab-vacuum interfaces can then be written for s polarization in the form

\[
A_n^{(s)} + B_n^{(s)} = C_n^{(s)} + D_n^{(s)} \quad \text{(III.11a)}
\]

\[
\left( A_n^{(s)} - B_n^{(s)} \right) \cos(\theta) = \sqrt{\varepsilon} \left( C_n^{(s)} - D_n^{(s)} \right) \cos(\theta_n) \quad \text{(III.11b)}
\]

and for p polarization in the form

\[
A_n^{(p)} + B_n^{(p)} = \left( C_n^{(p)} + D_n^{(p)} \right) \cos(\theta) \quad \text{(III.12a)}
\]

\[
A_n^{(p)} - B_n^{(p)} = \sqrt{\varepsilon} \left( C_n^{(p)} - D_n^{(p)} \right) \quad \text{(III.12b)}
\]

Applying these boundary conditions twice we can express the amplitudes \( A^{(s,p)} \) and \( B^{(s,p)} \) in the \( n-1 \)-th layer in term of the amplitudes \( A^{(s,p)} \) and \( B^{(s,p)} \) in the \( n \)-th layer. Specifically, for the electromagnetic field calculation in Eq. (III.11) and (III.12) this forms the basis of the transfer matrix method for the solution of the electromagnetic waves in the layered system. In our calculations we use the specific realization of the transfer matrix method developed in the Ref. [69]. We consider the system shown in Figure 8 where the \( n \)-th slab has a thickness \( b_n \) and the separation between \( n-1 \)-th and \( n \)-th slabs is \( a_n \). Applying the boundary condition in (III.11) or (III.12) for s and p polarizations receptively and using
(III.9) for the field inside the slabs or in the vacuum, we find the amplitudes of
the electric field $A_{n-1}$ and $B_{n-1}$ on the left side of the $n$-th slab are related to
those on the left side of $n + 1$-th slab by the linear transformation:

\[
\begin{pmatrix}
A_{n-1} \\
B_{n-1}
\end{pmatrix} =
\begin{pmatrix}
T_{11}(n) & T_{12}(n) \\
T_{21}(n) & T_{22}(n)
\end{pmatrix}
\begin{pmatrix}
A_n \\
B_n
\end{pmatrix}
\]

(III.13)

Here $T$ denotes the transfer matrix. Using (III.11), (III.12) and (III.9) we get
the following expressions for the elements of $T$.

\[
T_{11}^s(n) = \exp(iq_v a_n) \left[ \cos(q_m b_n) + \frac{i}{2} \left( \frac{q_m}{q_v} + \frac{q_v}{q_m} \right) \sin(q_m b_n) \right]
\]

(III.14a)

\[
T_{12}^s(n) = \exp(-iq_v a_n) \left\{ \frac{q_m}{q_v} - \frac{q_v}{q_m} \right\} \sin(q_m b_n)
\]

(III.14b)

\[
T_{21}^s(n) = T_{12}^{s*}(n)
\]

(III.14c)

\[
T_{22}^s(n) = T_{22}^{s*}(n)
\]

(III.14d)

for $s$ polarization and

\[
T_{11}^p(n) = \exp(iq_v a_n) \left[ \cos(q_m b_n) + \frac{i}{2} \left( \frac{q_v \varepsilon}{q_m} + \frac{q_m}{q_v \varepsilon} \right) \sin(q_m b_n) \right]
\]

(III.15a)

\[
T_{12}^p(n) = \exp(-iq_v a_n) \left\{ \frac{q_v \varepsilon}{q_m} - \frac{q_m}{q_v \varepsilon} \right\} \sin(q_m b_n)
\]

(III.15b)

\[
T_{21}^p(n) = T_{12}^{p*}(n)
\]

(III.15c)

\[
T_{22}^p(n) = T_{22}^{p*}(n)
\]

(III.15d)

for $p$ polarization.

The transfer matrix calculated above is the transfer matrix for one vacuum
layer and one dielectric slab. Subsequently, using (III.13) we find that the transfer
matrix $T$ for $N$ layers is given by
\[ T = \prod_{n=1}^{n=N} T(n) \quad \text{(III.16)} \]

In the case of a periodic system the \( T_{ij}(n) \) matrix does not depend on \( n \) and the product in (III.16) is equal to \( n \)-th power of \( T_{ij}(1) \). Because of the translation symmetry of the pure system by the distance \( a \) in the \( x \) direction, we can introduce the quasi wave vector \( \kappa \) then apply Bloch's theorem and obtain the band structure \( \omega(\kappa) \) of the system. In the disordered system, however, the \( T_{ij}(n) \) matrix does depend on \( n \) through the different values of slabs thickness. The disordered system does not have a translation symmetry by \( a \) in the \( x \) direction, and it is impossible to get a band structure like \( \omega(\kappa) \). We determine only if or if not light of the given frequency decays while propagates through the sample.

Now let us suppose that a plane wave of unit amplitude is incident from the left site of the sample. This means that \( A_0 = 1 \) and \( B_0 \) determines the reflection coefficient. Also we have that \( B_N = 0 \), because there is no reflected wave on the right edge. Hence

\[
\begin{pmatrix}
1 \\
B_0 \\
\end{pmatrix} = \begin{pmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22} \\
\end{pmatrix} \begin{pmatrix}
A_N \\
0 \\
\end{pmatrix} \quad \text{(III.17)}
\]

We then can obtain the reflection and transmission coefficients from Eqs. (III.17) and (III.9). We define the transmission coefficient as

\[
T = \frac{|S_x^{\text{trans}}|}{|S_x^{\text{inc}}|} \quad \text{(III.18)}
\]

which for an incident plane wave is equal to:

\[
T = \frac{1}{|T_{11}(k_x)|^2} \quad \text{(III.19)}
\]
\[ k_x = \frac{\omega}{c} \cos \theta_i \]  

(III.20)

III.4. Transmission Coefficient for a Beam

In this section we calculate the transmission coefficient for an incident beam (III.3) defined in accordance with (III.18). It can be calculated as follows. The \( x \) component of Poynting vector for \( s \)-polarized wave is equal to

\[ |S_x| = \frac{c^2}{4\pi \omega} \int \left| E(x, z) \frac{\partial E^*(x, z)}{\partial z} \right| dz \]  

(III.21)

Substituting (III.3) into (III.21) and performing integration over \( dz \) gives a delta-function, after which performing the integration over \( dq' \) we obtain:

\[ |S_x| = \frac{c^2}{4\pi \omega} \int \frac{dq}{2\pi} \sqrt{\left( \frac{\omega}{c} \right)^2 - q^2} |A(q)|^2 \]  

(III.22)

Performing the same procedure for \( p \)-polarized wave we obtain the same expression (III.22).

Now the transmission coefficient for a beam can be expressed as a superposition of planewave transmission coefficients weighted by \( \sqrt{\left( \frac{\omega}{c} \right)^2 - q^2} \).

\[ T = \frac{S_{\text{trans}}}{S_{\text{inc}}} = \frac{\int dq \sqrt{\left( \frac{\omega}{c} \right)^2 - q^2} |A(q)/T_{11}(k_x(q))|^2}{\int dq \sqrt{\left( \frac{\omega}{c} \right)^2 - q^2} |A(q)|^2} \]  

(III.23)

As mentioned above this form for the transmission coefficient is related to the conservation of wavevector for transmitted plane waves.
III.5. Localization Length Calculation

The localization length calculation is a very difficult problem in the case of two or three dimensional systems. In 1D case the localization length $\xi$ can be calculated much easier. There are two different methods to calculate the localization length in the 1D optical system. First one treats a complex refraction coefficient from which the localization length is obtained. Second one is to calculate the localization length by performing a statistical averaging of the transmission coefficient. We compute the localization length in a semi-infinite system for incident planewaves or for finite beams by using statistical averaging of the transmission coefficient.

The transmission coefficient in the 1D system is proportional to $T \propto \exp(-L/\xi)$ where $L$ is the system's total length. Consequently, $\xi \propto \frac{L}{\ln(T)}.$ This equation is valid for just one configuration. After applying configuration averaging we will get the final result for the localization length of the array. In 1D systems fluctuations in $T$ have a root of the mean square variance of order $T$. Because of this fact we have to perform a configuration averaging of the $\ln(T)$ as $\ln(T)$ exhibits a root of the mean square variance proportional to $1/\sqrt{N}$ where $N$ is the number of configurations averaged over.

The localization length $\xi$ of our random slab system is related to the transmission coefficient and is defined by

$$\xi = -\frac{L}{\langle \ln T \rangle} \quad (\text{III.24})$$

where $L$ is total length of the array of slabs and $\langle \cdot \rangle$ indicates a configuration average over random configurations of our slab system.

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III.6. 1D Results

In the Figures 9a and 9b we present results for the localization length along the x-axis of the electromagnetic field versus $a/\lambda$ for planewave incident on the system defined in (III.1). Results are shown for $\theta = 0^\circ, 40^\circ, 60^\circ$ and $71^\circ$. The Ioffe–Rigel parameter $\xi \omega / c$ is computed as a function of inverse wavelength $a/\lambda$. These results were obtained for the case of incident planewaves by computing the transmissivity, $T$, of systems consisting of finite arrays of $N = 57$ slabs. The localization length, $\xi$, is defined by (III.24). In general, from 100 to 200 different configurations were used in the determination of $\xi$. We present results for $\xi \omega / c$ versus $a/\lambda$ for $\theta_i = 0^\circ, 40^\circ, 60^\circ$ and $71^\circ$. These are computed for the slab system defined in Eq. (III.1). The localization length exhibits small values within the stop bands of the periodic (i.e. $f_n = 0$) system. The stop bands of the $f_n = 0$ system $0.22 \leq a/\lambda \leq 0.44$ for $\theta_i = 0^\circ$, $0.22 \leq a/\lambda \leq 0.46$ for $\theta_i = 20^\circ$, $0.23 \leq a/\lambda \leq 0.52$ for $\theta_i = 40^\circ$, $0.24 \leq a/\lambda \leq 0.63$ for $\theta_i = 60^\circ$, $0.24 \leq a/\lambda \leq 0.67$ for $\theta_i = 71^\circ$ and for $p$-polarization are $0.22 \leq a/\lambda \leq 0.44$ for $\theta_i = 0^\circ$, $0.23 \leq a/\lambda \leq 0.45$ for $\theta_i = 20^\circ$, $0.28 \leq a/\lambda \leq 0.48$ for $\theta_i = 40^\circ$, $0.4 \leq a/\lambda \leq 0.51$ for $\theta_i = 60^\circ$ and there is no stop band for $p$-polarized plane wave incident at $\theta_i = 71^\circ$. Within the stop bands the localization lengths are of order of just a few multiples of $a$. An exception to this is observed for $p$-polarization in which the localization length diverges at the Brewster’s angle, $\theta_{br} = 71.6^\circ$. The divergence of the localization length for $p$-polarization at the Brewster’s angle was noted in Ref. [55]. In general, however, the $p$-polarization localization length is found to be larger than the $s$-polarization localization length computed for the same wavelength and incident angle.
Figure 9.  (a) Localization Length for the $s$ Polarized Plane Waves Versus $a/\lambda$.  (b) Localization Length for the $p$ Polarized Plane Waves Versus $a/\lambda$.  (c) Angular Dependence of the Localization Length for Plane Waves With $a/\lambda = 0.3385$ for $s$ Polarization (Solid) and for $p$ Polarization (Dashed).
Figure 10. The Dependence of the Localization Length on the Strength of the Disorder $\delta a$ for $s$ Polarized Wave (Solid) and for $p$-Polarized Wave (Dashed) for $\theta = 45^\circ$ and $\theta = 60^\circ$.

To illustrate the angular dependence of the localization length in the Figure 9c we present results for $\xi \omega/c$ versus $\theta_i$ for $a/\lambda = 0.3385$ which is a value of $a/\lambda$ that falls near the center of the $\delta a = 0$ band gap for both $s$ and $p$ polarizations at quite general values of $\theta_i$. The smaller localization length of $s$ polarization system are readily seen from these plots. And the localization length for $p$ polarized wave increases with the increasing of the incident angle and is equal to infinity at Brewster angle. This correspond to results of Ref. [55]. In general, for the successful numerical simulation of Anderson localization phenomena, systems chosen for study must have the smallest possible localization lengths. This will be of particular importance in the $R$-matrix calculations of beam spreading presented below and is the basis of our choice of $a/\lambda = 0.3385$ in this work.

In the Figure 10 we present the results the dependence of the localization local on the strength of the disorder. The results are presented for $a/\lambda = 0.3385$ plane wave incident at $\theta_i = 45^\circ$. The value of the disorder was changed by changing the value of $\delta a$ in (III.1) from 0 to 0.25. The results are presented for
Figure 11. The Dependence of the Localization Length $\xi_\omega/c$ on $a/\lambda$ for
$p$–Polarized Beam With $\varpi = 3\lambda, 5\lambda, 20\lambda$ and for the Plane Wave.

two incident angles: $\theta = 45^\circ$ and $\theta = 60^\circ$ We see that the localization length
for $s$ polarized plane does not exhibit significant dependence on the strength of
the disorder. In the same time $p$ polarized wave exhibit significant dependence
of the localization length on the disorder. The localization length increases for
$\theta = 45^\circ$ and decreases for $\theta = 60^\circ$ with the increase of the disorder. Such different
dependence is caused by two effects: the direct influence of a disorder on the
localization length and indirect influence through shifting of the stop–bands in
the system. The results when the localization length increases with the increasing
of the disorder also been obtain in Refs. [11,38] for a different system.

To show the importance of the divergence of the localization length for $p$–
polarization at the Brewster's angle, we considered a Gaussian beam with
$A(q)$ from (III.6) which is incident at $\theta = 60^\circ$ (that is close to Brewster's angle
$71.6^\circ$). In Figure 11 we present the localization length along the $x$–axis for the
$p$–polarized Gaussian beam as a function of inverse wavelength $a/\lambda$. We present
the results for the beams with the width $\varpi = 3\lambda, 5\lambda, 20\lambda$ and for the incident
plane wave. The beams with small width are seen to exhibit larger localization

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lengths because of the significant presence of Brewster's angle components. The localization lengths for wide beams are close to those for incident plane wave. The $s$-polarized waves do not exhibit that anomaly and the localization length for a finite incident beam is similar to one for a plane wave. For $\theta_i \approx \pi/2$ we also observed transverse localization effects (beam spreading) similar to those observed by De Raedt, et al [52].

While the localization length describes roughly statistical properties of the distribution of electromagnetic intensity in space, a direct calculation of the electromagnetic field can be made for a single sample. This shows directly a typical field distribution in space. For the incident planewave case, Eq. (III.2), the field intensity in the slabs depends only on $x$. In the beam case, Eq. (III.3), however, the localized beam exhibits both $x$ and $z$ dependence, and for this case we present results for the field intensity as a function of $x$ at various fixed values of $z$. This second case, then, is closest to the original study of De Raedt, et al [52]. We have considered a beam of the form of Eq. (III.3) incident on our array of slabs. Results for this system can be obtained as a Fourier transform involving the planewave results in Eq. (III.3). In particular, we have studied the beam spreading in the $x$-direction as a function of the propagation of the beam in the $z$-direction. A number of angles of incidence $\theta_i$ were considered. The spreading of the beam is found to closely correlate with the localization lengths in Figure 9.

In Figure 12 we present, for a finite incident beam plots of $|E(x, z)|$ versus $x$ for $z = 0, 20a, -20a$ and $50a$. The wavelength of light in our system was chosen to be in a stop band of the $\delta a = 0$ system with $a/\lambda = 0.3385$ as this condition is known to facilitate the observation of small localization lengths in the $\delta a = 0$ system. Results are shown for both $s$- and $p$-polarized beams with
\( \omega = 3 \lambda \) for \( \theta_i = 60^\circ \). In the case of \( s \)-polarization the beam is found to be limited in its spreading to a width at half maximum which is roughly given by the localization length in Figure 9. The \( p \)-polarization, however, is found not to exhibit localization effects at \( \theta_i = 60^\circ \) that is close to Brewser angle 71.6°. At this angle the maximum of field distribution occurs at the points on the lines in the center of the beam.

This absence of localization is due to the presence of a large amount of Brewster angle components in the beam. These modes are not localized. Runs at \( \theta_i = 0^\circ, 20^\circ \) and \( 45^\circ \) for \( p \)-polarization were made for the beam in Eq. (III.3) and were found to be localized with a localization length similar to that in Figure 9 for these incident angles. These beams contained negligible amounts of Brewster angle components.

III.7. Transverse Localization Effects in 2D Layered Systems

The system we study in this section consists of an array of dielectric rods of square cross section in vacuum which are translationally invariant in the \( z \) direction and which form a square lattice in the half-plane of \( x - y \) plane defined by \( x > 0 \). The rods are formed of randomly disordered dielectric material with a dielectric constant which depends only on \( x \) and \( y \). The semi-infinite square lattice array of rods is then described by the dielectric constant:

\[
\varepsilon(x, y) = \begin{cases} 
\varepsilon + \delta \varepsilon(x, z), & (n + 0.5)a - d/2 \leq x \leq (n + 0.5)a + d/2 \\
(m + 0.5)a - d/2 \leq y \leq (m + 0.5)a + d/2 \\
1, & \text{otherwise}
\end{cases} \tag{III.25}
\]

where \( n, m = 0, 1, 2, \ldots \); \( a \) is the lattice constant; \( d \) is the length of a size of the
Figure 12. Electric Field for $\omega = 3\lambda$ Beam With $\theta_i = 60^\circ$ Versus $x/a$ for $z = 0, -20a, 20a$ and $50a$. (a) $s$ Polarization, (b) $p$ Polarization.

rods in the $x-y$ plane; $\epsilon$ is the average dielectric constant of the rods; and $\delta \epsilon(x, y)$ is a small zero mean random fluctuation which we discuss below.

The light incident on this system is a plane wave propagating in the $x-z$ plane and incident from the region $x < 0$. We will be interested in computing the localization length of light measured along the $x$ axis. This is done as in the layered system by computing the transmissivity for an array of finite length $L = Na$ along the $x$ axis and studying the behaviour of the transmissivity as a
function of $L$. We define the localization length in similar way as we did in the case of 1D system (III.24). Specifically, we define the transmission coefficient as:

$$T = \frac{|S_{z}^{\text{transm}}|}{|S_{z}^{\text{inc}}|} \quad (\text{III.26})$$

where $S_{z}^{\text{transm}}$ and $S_{z}^{\text{inc}}$ are $z$ components of Poynting vector of transmitted and incident planewaves, respectively. The localization length $\xi$ can be defined by analogy with the 1D case [29,54,56]:

$$\xi = - \frac{L}{\langle \ln T \rangle} \quad (\text{III.27})$$

The definition (III.27) is differs by the factor of 2 from the definition of the localization length in the 1D case [54,56] in Eq. (III.24). This definition of the transverse localization length (III.27) obeys all the usual properties of the localization length and can be applied to study transverse localization in the 2D systems.

The 2D system we have defined in Eq. (III.25) has the advantage of being an almost periodic system. This means that the localization length for frequencies in the stop bands of the $\delta\varepsilon(x,y) = 0$ system should be very small. This facilitates their numerical simulation. In particular, for cases in which the localization length $\xi$ is smaller than a lattice constant, we expect that the differences in $\delta\varepsilon(x,y)$ between different rods in the system should have a small effect on the value of $\xi$. Consequently, in the results presented below we will assume that $\delta\varepsilon(x + la, y + ma) = \delta\varepsilon(x, y)$ for $l, m = 0, \pm 1, \pm 2, \ldots$

To treat this periodic system we used the theory and the program of Ref. [6]. The geometry we study is shown if Figure 13. The elementary cell is covered by 12x12 mesh and we set the dielectric constant in the each point of this cell. In
the center of the cell (point from 4 to 9 of the mesh in $x$ and $y$ directions) there is a square rod. The dielectric constant in these points was chosen as $\epsilon_{ij} = \epsilon + \delta \epsilon f_{ij}$ where $\epsilon = 9$, $\delta \epsilon = 1$ and $f_{ij}$ is a random number uniformly distributed over the interval $-1 \leq f_{ij} \leq 1$. The system consists of 20 cells in $x$ direction and infinite number of cells in $y$ direction. This dielectric structure was treated by using the program of Ref. [6].

III.7.1. 2D Transfer Matrix

The 2D transfer matrix approach of Ref. [6] considers the case when a plane wave with the wavevector $(k_x, k_y, k_z)$ is incident on a periodic 2D system with the periods $a$, $b$ and $c$ in the $x$, $y$ and $z$ directions respectively. This approach starts with the Maxwell equations (III.8) and is based on following approximation:

$$k_x \approx \frac{\exp(i k_x a) - 1}{i a}$$

(III.28a)
the approximation (III.28) when applied to Maxwell equations allows us to express all space derivative by a finite difference. After applying the approximation (III.28) in Maxwell equations (III.8) and eliminating the $E_z$ and $H_z$ components we can express the field in the $r+c$ points in terms of field in the $r$ points.

$$F(z + c) = TF(z)$$  \hspace{1cm} (III.29)

where $F(z_0)$ is the vector of all $E_x$, $E_y$, $H_x$ and $H_y$ in all the points at the plane $z = z_0$.

The equation (III.29) defines the transmission coefficient in a basis chosen to facilitate the numerical integration. To obtain the transmission coefficient for a plane wave we used the procedure of Ref. [6]. Specifically, we transform the matrix $T$ to the basis of its left- and right- eigenvectors. In this new basis the transmission coefficient can be calculated for a plane wave. The above described procedure, because of numerical instability, can be applied only to one cell. After obtaining the transfer matrix for one cell we can apply standard multiple scattering mechanism to obtain the transfer matrix for two cells, etc. Specifically we used the approach of Refs. [6,49] for calculation of transfer matrix for entire sample.

III.8. 2D Transverse Localization. Results

In Figure 14a we present results for the localization length along the $z$-axis of the electromagnetic field in the case of a normal incident plane wave. The
Ioffe–Rigel parameter $\xi \omega / c$ is computed as a function of inverse wavelength $a / \lambda$. These results were obtained for the case of incident planewaves by computing the transmissivity, $T$, of systems consisting of finite arrays of $N = 20$ layers of rods. The transverse localization length, $\xi$, is defined by (III.27). In general, from 50 to 100 different configurations were used in the determination of $\xi$. It should be noted, that in contrast with 1D results in the 2D system the separation on $s$ and $p$ polarization cases is possible only for an incident wave with $k$ in $x - y$ plane. For off-angle incidence we have two different modes that we cannot label as $s$ and $p$ polarizations. From this graph we see that in the 2D case there is a strong difference in localization length for $s$ and $p$ polarized waves ever for normal incidence.

In contrast with the 1D case, in the 2D case the light scattering exhibit significant polarization dependence in the case of normal incidence (for example they have different stop bands). This difference is seen in the Figure 14a.

In the Figure 14b we present the localization length for a plane wave incident at Brewster angle $\theta = 71.6^\circ$. The two curves represent two modes, that cannot be classified as $s$ and $p$ polarization. These modes are the linear combination of $s$ and $p$ polarizations. A direct expression for this linear combination can be obtained by diagonalization of $T$ matrix for one layer in (III.29) and then calculating the $T$ matrix for several layers. The major difference between the 1D and 2D cases is the absence of Brewster angle singularity in the 2D case. This singularity is absent because of the absence of translation symmetry in two directions.
Figure 14. Localization Length $\xi \omega / c$ Versus $a / \lambda$ for 2D System. (a) for $\theta = 0^\circ$, s Polarization (Solid Line) p Polarization (Dashed Line). (b) for $\theta = 71^\circ$ Solid and Dashed Lines – Two Different Modes (Both Modes Are a Superposition of s and p Polarized Waves.

III.9. Conclusion

In this chapter we considered the transverse localization of light. We applied the full 3D Maxwell's equations treatment in this study. We considered 1D and 2D cases. In the 1D case we studied a semi–infinite array of dielectric slabs separated by vacuum in the case of incident plane waves and an incident beam of light. We showed that the transverse localization length exhibits strong
polarization dependence. The $s$ polarized waves usually are better localized than the $p$ polarized waves. In the case of an incident beam of $p$ polarized waves the transverse localization length exhibits a strong dependence on beam’s width. This dependence is caused by a Brewster angle anomaly and the fact that the amplitude of beam’s components at Brewster angle depends on the beam’s width. The transverse localization length for an $s$ polarized incident beam is similar to one of the incident plane wave and does not exhibit a significant dependence on beam’s width.

In the 2D case we studied a system that consisted of a semi-infinite array of infinite rods with the incident plane waves. The 2D system exhibits a strong polarization dependence of its localization length in the case of normal incident waves. One more important difference between 2D and 1D systems is the absence of a Brewster angle anomaly in the 2D case. This difference is caused by the difference in the symmetry of the two problems.
CHAPTER IV

DETERMINATION OF SURFACE PROFILE STATISTICS FROM ELECTROMAGNETIC SCATTERING DATA

IV.1. Introduction

A new method known as reverse Monte Carlo (RMC) has recently been developed and applied to the determination of the structures of amorphous and polymer materials from X-ray scattering data [36]. This method uses Monte Carlo techniques to generate atomic structures which reproduce the scattering data obtained experimentally from disordered systems, and hence act as models for the atomic arrangement in these materials. In this dissertation we present a new application of RMC ideas, namely the determination of the power spectrum of a randomly rough surface from the differential reflection coefficient of electromagnetic radiation scattered from such a surface, i.e. from far-field experimental data.

In contrast with the standard Monte Carlo approach, where for a given statistical distribution of random configurations one calculates some physical value, in the Reverse Monte Carlo simulations for a given physical value (in our case this is the differential reflection coefficient) we calculate the statistics of random surfaces. This approach originates from the work by McGreevy and Howe. They applied it to the determination of the structures of amorphous and polymer materials from X-ray scattering data [36]. We apply the RMC method to the determination of the surface profile statistics from the scattering data.

The RMC method works as follows: First the RMC employs Monte Carlo
techniques in which various surface statistics (i.e. the power spectrum of the surface roughness) are randomly generated. Then the Differential Reflection Coefficient that describes the angular distribution of the scattered field for these simulated surface statistical properties, is calculated. Perturbation theory or direct numerical simulation is used to compute the differential reflection coefficient for the given surface power spectrum. Next the RMC employs a maximal entropy approach that allows for the determination from the generated surface statistics of those statistics that best fit the experimental data. This allows us to sort out previously generated surface statistics and construct new surface statistics from those saved. We continue the above RMC procedure with the scattering data to fit the differential reflection coefficient from the generated surface statistics to the scattering data. After a number of such steps we can obtain surfaces with statistics that match the experimental data.

We study a 1D random surface with the surface profile \((x_1, 0, \zeta(x_1))\), Figure 15, and treat the height \(\zeta(x_1)\) as a Gaussian random process. Specifically,

\[
\langle \zeta(x_1) \rangle = 0 , \tag{IV.1a}
\]

\[
\langle \zeta(x_1) \zeta(x_1') \rangle = \sigma^2 W(x_1 - x_1') \tag{IV.1b}
\]

with the autocorrelation function \(W(x_1)\) and \(\langle \cdots \rangle\) represents an average over a set of surface profiles. The power spectrum of the surface roughness \(g(k)\) is defined as the Fourier transform of \(W(x_1)\)

\[
g(k) = \int dx_1 \exp(-iqx_1)W(x_1) \tag{IV.2}
\]

We introduce the functional \(\chi\) defined below. This functional determines
the difference between measured differential reflection coefficient (DRC) and the differential reflection coefficient calculated from the generated statistics \( g(k) \). The problem of fitting the surfaces statistics is in fact a problem of finding the most probable minimization of \( \chi \) subject to the experimental data and its error. Specifically, we define

\[
\chi = \sum \sum \int d\Omega_s [\sigma(\Omega_l, \Omega_s) ]^{-2} \\
\times \left| \left( \frac{dR_{\alpha,\beta}(\Omega_i, \Omega_s)}{d\Omega_s} \right)_{\text{exp}} - \left( \frac{dR_{\alpha,\beta}(\Omega_i, \Omega_s)}{d\Omega_s} \right)_{\text{theory}} \right|^2,
\]

where \( \left( \frac{dR_{\alpha,\beta}(\Omega_i, \Omega_s)}{d\Omega_s} \right)_{\text{exp}} \) is the experimentally measured differential reflection coefficient, \( \left( \frac{dR_{\alpha,\beta}(\Omega_i, \Omega_s)}{d\Omega_s} \right)_{\text{theory}} \) is the differential reflection coefficient calculated by

Figure 15. Scattering of Light on a Random Surface.
theory for a given $g(k)$ statistics and $\sigma(\Omega_i, \Omega_s)$ is proportional to the experimental errors. The indices $\alpha, \beta = 1, 2$ label $s$ and $p$ polarization respectively, the $\Omega_i$ are angles of incidence and $\Omega_s$ are scattered angles. The sum on $i$ allows for the use of scattering data from more than one angle of incidence. The exact power spectrum $g^{(0)}(k)$ gives $\chi = 0$ when substituted into the RMC as a guess. The plane of incidence is assumed to be the $x_1x_2$-plane, and the incident light is $p$-polarized. In this scattering geometry there is no cross-polarized scattering.

Next we have to transform the problem of finding the most probable minimization of $\chi[g(k)]$, consistent with the experimental data and its errors, on some set of functions $\{g(k)\}$, to the problem of determining the most probable $g(k)$ to match the measured DRC. Instead of one function $g(k)$ we here introduce an ensemble of $\{g_i(k)\}$ which are generated by random process, each realization of which gives us a possible $g(k)$. $\chi[g(k)] \equiv 0$ if $g(k)$ reproduces exactly the experimental spectra. Each realization of $\{g_i(k)\}$ gives some value $\chi_i$. Now we can study $\{g_i(k)\}$ as $g^{(0)}(k) + \{e_i(k)\}$ where $\{e_i(k)\}$ serves as "experimental errors" in the problem and $g^{(0)}(k)$ is the best $g(k)$ to fit the data. We then use the maximum entropy approach to find the most probable solution for $g(k)$ consistent with experimental data including the error limits of the experimental data. For this state the entropy of the probability distribution of $\chi$ takes its maximal value.

We are looking for surface statistics $g^{(0)}(k)$ that are the most probable, i.e. minimizing $\chi$ while maximizing the entropy of the distribution of $\chi$. Entropy is a concept in probability theory and the maximum entropy method is applicable when we are determining a function such as $\chi$ that is distributed by some probability distribution.

The probability of each particular $\chi$ configuration studied in our RMC is
given by the Boltzmann’s formulae:

\[ P \propto \exp(-\chi) \]  

(IV.4)

Eq. (IV.4) follows from the maximal entropy theory, and it has the same meaning as it has in the statistical mechanics theory of the determination of the state of a thermodynamic system in contact with a constant temperature bath. The probability from (IV.4) satisfies the following basic relation:

\[ P(\chi_1 + \chi_2) = P(\chi_1)P(\chi_2) \]  

(IV.5)

which reflects that fact that entropy \((-P \log P)\) is an extensive value.

The RMC method when applied to optical scattering data from rough surface operates essentially the same as the Monte Carlo study of a thermodynamic system based on the Boltzmann probability distribution.

Our method works as follows:

1. We take an initial guess \(g_0(k)\), which yields a differential reflection coefficient \((dR_{\alpha,\beta}(\Omega_i, \Omega_s)/d\Omega_s)\_0\), and a \(\chi_0\). The initial configuration can be chosen in any manner. The probability of the \(g_0(k)\) configuration being a good representation of our surface is \(P_0\) given by Boltzmann’s formulae (IV.4).

2. A random change is then made in \(g_0(k)\) to create a new guess power spectrum \(g_1(k)\), which yields a new differential reflection coefficient \((dR_{\alpha,\beta}(\Omega_i, \Omega_s)/d\Omega_s)\_1\), and a new value of \(\chi, \chi_1\). The probability that this \(g_1(k)\) is a good representative of our surface configuration is given by Boltzmann’s formulae (IV.4). Then

\[ p = P_1/P_0 = \exp(-\chi_1 - \chi_0) \]  

(IV.6)
3. If $x_1 < x_0$ then $g_1(k)$ is retained over $g_0(k)$ as a good guess for the power spectrum. If $x_1 \geq x_0$ then $g_1(k)$ is retained over $g_0(k)$ with probability $p = \exp(x_0 - x_1)$. This last step keeps the system from becoming stuck in a local minimum of $x_1$, and helps us choose the most probable solution for $g(k)$ consistent with the experimental data. Otherwise, $g_0(k)$ is retained, and the above process is repeated until $(dR_{\alpha\beta}(\Omega_1, \Omega_2)/d\Omega_2)^\exp$ agrees with $dR_{\alpha\beta}(\Omega_1, \Omega_2)/d\Omega_2$ from theory.

The final guess for $g(k)$ is taken to represent the true power spectrum. In view of the Monte Carlo sampling on which the RMC method is based, we expect that it converges to the true power spectrum with an error that decreases inversely with the square root of the number of Monte Carlo comparisons used.

We apply the method just described to the determination of the power spectrum of weakly rough, one-dimensional, random metal surfaces (i.e. surfaces for which $\langle x_\parallel \rangle$ is independent of $x_2$), for which an analytic expression for the mean differential reflection coefficient in terms of the power spectrum exists [37]. It has been obtained by an infinite-order perturbation calculation in the small roughness approximation [64]. The plane of incidence is assumed to be the $x_1x_3$-plane, and the incident light is p-polarized. In this scattering geometry there is no cross-polarized scattering. The contribution to the mean differential reflection coefficient from the diffuse component of the scattered light is related to the power spectrum $g(k)$ by [37]

$$
\langle \partial R_p(\theta_s, \theta_t)/\partial \theta_s \rangle_{\text{diff}} = \frac{\omega}{4\pi^2c} \cos \theta_s (I^{(L)}(q|k) + I^{(c)}(q|k)), \quad (IV.7)
$$

where $q = \frac{\omega}{c} \sin \theta_s, k = \frac{\omega}{c} \sin \theta_t$. The values of $I^{(L)}(q|k)$ and $I^{(c)}(q|k)$ are related.
to the ladder and crossed term respectively [37]. They are given by

\[ I^{(L)}(q|k)_{\text{diff}} = 8\pi\alpha_0(q)\alpha_0(k)|G(q)|^2|G(k)|^2 \]

\[ \times \left[ K(q, k) + \frac{C^2_1}{2\Delta_{\text{tot}}} \frac{1}{1 - \left( \frac{\Delta_{\text{sp}}}{\Delta_{\text{tot}}} \right)^2} \left\{ K(q, K_{\text{sp}})K(K_{\text{sp}}, k) + K(q, -K_{\text{sp}})K(-K_{\text{sp}}, k) \right. \right. \]

\[ + \frac{\Delta_{\text{sp}}}{\Delta_{\text{tot}}} \left( K(q, K_{\text{sp}})K(-K_{\text{sp}}, k) + K(q, -K_{\text{sp}})K(K_{\text{sp}}, k) \right) \left. \right\} \]  

\[ \text{(IV.8)} \]

\[ I^{(c)}(q|k) = 8\pi\alpha_0(q)\alpha_0(k)|G(q)|^2|G(k)|^2 \]

\[ \times \frac{4\Delta_{\text{tot}}C^2_1}{(q + k)^2 + 4\Delta^2_{\text{tot}}} \frac{1}{1 - \left( \frac{\Delta_{\text{sp}}}{\Delta_{\text{tot}}} \right)^2} \]

\[ \times \left[ K(k, K_{\text{sp}})K(k, -K_{\text{sp}}) + \frac{\Delta_{\text{sp}}}{2\Delta_{\text{tot}}} \{ K^2(k, K_{\text{sp}}) + K^2(k, -K_{\text{sp}}) \} \right] \]  

\[ \text{(IV.9)} \]

where

\[ K(q, k) = \left| \frac{\epsilon(\omega) - 1}{\epsilon^2(\omega)} \right|^2 |\epsilon(\omega)qk - \alpha(q)\alpha(k)|^2 g(|q - k|) \]  

\[ \text{(IV.10)} \]

\[ K(q|k) = \delta^2 g(q - k)|\epsilon(\omega) - 1|/\epsilon^2(\omega)^2 |\epsilon(\omega)qk - \alpha(q, \omega)\alpha(k, \omega)|^2 \], with \( \epsilon(\omega) \) the dielectric function of the metal; \( \alpha(q, \omega) = [\epsilon(\omega)/(\omega/c)^2 - q^2]^{1/2} \), \( \text{Re}\alpha(q, \omega) > 0, \text{Im}\alpha(q, \omega) > 0 \); and \( \Delta_{\text{sp}} \) in Eqs. (35) and (45) of Ref. [37] is defined by \( \Delta_{\text{sp}} = 2\pi\delta^2C^2_1[(\epsilon^1(\omega) - 1)/\epsilon^1(\omega)]^2 k^4_{\text{sp}}(\omega)g(2k_{\text{sp}}(\omega)) \), where \( C_1(\omega) = (-\epsilon^1(\omega))^{3/2}/[\epsilon^2(\omega) - 1] \), \( k_{\text{sp}}(\omega) = (\omega/c)[\epsilon^1(\omega)/(\epsilon^1(\omega) + 1)]^{1/2} \), and \( \epsilon^1(\omega) = \text{Re}\epsilon(\omega) \).

IV.2. Results

We have used the theoretical results of Ref. [37] to generate “experimental” mdrc data for the scattering of p-polarized light of wavelength \( \lambda = 457.9nm \) from a silver surface \( \epsilon(\omega) = -7.5 + i0.24 \) characterized by the power spectrum \( g(k) = \sqrt{\pi}a\exp(-k^2a^2/4) \), with roughness parameters \( \delta = 5nm \) and \( a = 100nm \).
The angles of incidence were arbitrarily chosen to be \( \theta_i = 10^\circ \), and \( 18^\circ \). The RMC method was then used to extract \( g(k) \) from these data. In order to use the least amount of \textit{a priori} information about the power spectrum, the initial guess for \( g(k) \) in the RMC reconstruction from the scattering data was \( g(k) = 0 \), and in making subsequent guesses we used the general properties \( g(k) \geq 0 \) and \( g(-k) = g(k) \). For \( k \) in the interval \( (0, 2.95(\omega/c)) \), \( \delta^2 g(k) \) was broken up into a histogram with 200 channels, and was allowed a random change in one channel for each Monte Carlo comparison described above. For \( k > 2.95(\omega/c) \) the value of \( g(k) \) does not affect the computed mdrc, so we took \( g(k) \equiv 0 \) in this region. A total of 20,000 Monte Carlo comparisons was used in obtaining the reconstructed power spectrum depicted in Figure 16, where it is compared with the exact power spectrum \( g(k) \) used in generating the "experimental" data. These calculations required 33 minutes of CPU time on a VAX 6000-620. Good agreement between the exact and reconstructed power spectra is observed, although better agreement could be obtained with longer runs.

As a stringent test of the effectiveness of the RMC method for recovering the \( g(k) \) from scattering data, we have applied it to scattering data recently measured by West and O'Donnell [67]. These authors fabricated a weakly rough, one-dimensional, random gold surface and measured the contribution to the mdrc from the incoherent component of the scattered light for p-polarized light of wavelength \( \lambda = 612 \mu m \) incident at \( 0^\circ \), \( 10^\circ \), and \( 18^\circ \) from the normal to the mean surface. The surface was fabricated in a manner that assured that the surface profile would obey Gaussian statistics.

As the surface studied in Ref. [67] is a weakly rough surface, we used in our RMC method the perturbation theory of McGurn \textit{et al.} [37] to express the
differential reflection coefficient in terms of the guessed \( g(k) \). In Figure 17 we present the results in dimensionless units for \( g(k) \) versus \( c k / \omega \) obtained in Ref. [67] by contact profilometry and by our application of the RMC method discussed above. The RMC result for \( g(k) \) was obtained by using the scattering data in Figure 16 of Ref. [67] for angles of incidence \( \theta_i = 10^\circ \) and \( 18^\circ \). Again, the initial guess for \( g(k) \) was taken to be \( g(k) \equiv 0 \), and 20,000 Monte Carlo comparisons were used. In presenting both sets of data we have taken \( \delta = 109\text{Å} \), which is the value obtained in Ref. [67] for this parameter. The value of \( \delta \) is used to normalize the power spectrum and does not affect the RMC computation of \( g(k) \). Good agreement is observed between our RMC results and the profilometry results.

For the results in Figures 16 and 17 no values of \( \sigma(\theta_i, \theta_a) \) were available. In such cases, by trial and error we choose \( \sigma \) small enough to reproduce the published data closely, but large enough to allow the maximum entropy component of our

Figure 16. Plot of \( g(k) \) Versus \( ka \). "Experimental" Power Spectrum (Dashed Line) \( g(k) = \sqrt{\pi} a \exp(-(ka)^2/4) \), and the RMC Extraction of it (Solid Line).
computer routine to operate efficiently. In the present case we chose \( \sigma(|\theta_s| \leq 80^\circ, \theta_i) = 10^{-6}\text{rad}^{-1} \), and \( \sigma(|\theta_s| \geq 80^\circ, \theta_i) = 10^{-5}\text{rad}^{-1} \). Scattering data for \( \theta_i = 10^\circ \) and \( 18^\circ \) were necessary to obtain accurate RMC results for \( g(k) \).

Although clearly much can be done to improve the efficiency of the method, we have demonstrated how RMC techniques can be used to extract the power spectrum of a randomly rough surface from measured results for the mdrf of light scattered diffusely from randomly rough surfaces. Existing methods for obtaining the power spectrum from diffuse scattering data (see, e.g. Ref. [62]) are based on a single-scattering approximation to the mdrf, which could not be used in reconstructing the West-O'Donnell power spectrum, because it produces surfaces from which single scattering processes are largely suppressed [67]. The RMC method in the present work is based on a multiple-scattering theory. As a result, the power spectrum \( g(k) \) can be obtained for a larger range of \( k \) than is possible.
with a single-scattering theory.

In addition, the RMC method contains two important improvements over routines which compute $g(k)$ by a straightforward minimization of $\chi$ [10]: (1) the Monte Carlo component of the RMC offers an efficient way to minimize $\chi$ approximately, (2) the maximum entropy component of the RMC sorts out from all of the local minima of $\chi$ the most probable solution for $g(k)$. In this regard, the more scattering data (more experimental points and more angles of incidence) used, the more probable is the agreement of the $g(k)$ computed by the RMC with the actual $g(k)$. It is important along with a study of the convergence of the RMC routine itself to study the change in the computed $g(k)$ as data from additional angles of incidence are added.

The method we have presented is readily generalized to treat surfaces which are defined by surface profile functions that are not Gaussian random processes. One generalization of the RMC method is the extraction of deterministic surface profiles from scattering data. In this work the differential reflection coefficient is expressed in terms of the surface profile function $\zeta(x_\|)$, and the random guesses in the RMC method are made of $\zeta(x_\|)$ rather than of the power spectrum as in the random surface RMC.

In the case that an analytic result for $\langle \partial R(\theta_s, \theta_i)/\partial \theta_s \rangle_{\text{diff}}$ is not available, the RMC method can still be used to determine the power spectrum $g(k)$, at the expense of additional computational effort. For each choice of $g(k)$ an ensemble of several hundred profiles would have to be generated by a standard method [34,44,63,65,66], the results for $\partial R(\theta_s, \theta_i)/\partial \theta_s$ for each member of the ensemble would have to be averaged, and the result used in the RMC algorithm.
CHAPTER V

SPECKLE CORRELATION STUDY OF LIGHT MULTIPLY SCATTERED
FROM RANDOMLY ROUGH METAL SURFACES

V.1. Introduction

When light scatters from a random surface we see in the scattered light a grainy structure of bright and dark spots. This grainy pattern in intensity of scattered light is known as speckle.

Figure 18. Grainy Structure in the Scattered Light.

The origin of speckle is in phase interference in the light scattered from the rough surface. The speckle correlation of light (i.e., the intensity correlations Figure 18) scattered at two different angles is the subject of our study in this chapter. As in the Chapter IV we study a 1D random surface, shown in the Figure 19, with the surface profile \((x_1,0,\zeta(x_1))\) and treat the height \(\zeta(x_1)\) as a Gaussian random process

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There is only one significant difference between the systems we study here and those we studied in Chapter IV. Now we have two beams that are incident on the random surface at two different incident angles. The angular correlation of the scattered light from these two beams is the subject of our study.

\[ \langle \zeta(x) \rangle = 0 \quad \text{(V.1a)} \]
\[ \langle \zeta(x) \zeta(x') \rangle = \sigma^2 W(x - x') . \quad \text{(V.1b)} \]

Figure 19. A Geometry for the Speckle Correlation Experiment.

The angular correlation study of light scattered from random media and rough surfaces has been of growing interest in the past decade [13,22,40,45,47]. Most of these studies were made in the context of a first order perturbation theory or Kirchhoff approximation treatment of the scattering of light. These approximations are equivalent to the single scattering approximation and give only memory and reversed memory effects in the angular intensity speckle correlator, denoted as the \( C^{(1)} \) correlator. Recent multiple-scattering theories of the angular intensity correlation functions for electromagnetic waves scattered from disordered volume systems have led to the prediction of a number of novel features [3,25,28,46] some
of which have been observed experimentally [25,28]. These features include long
range correlations, denoted $C^{(2)}$; and infinite range correlations, denoted $C^{(3)}$.
These new features have not been studied in surface scattering until the present-
tation of our treatment of these and other new correlators below.

In this chapter we study, for light scattered from a rough metal surface,
the angular correlator defined as follows:

$$C(q, k|q', k') = \left\langle \frac{I(q|k) - < I(q|k) >}{I(q'|k') - < I(q'|k') >} \right\rangle$$  \hspace{1cm} (V.2)

where $k$ and $k'$ are the wavevectors of two incident plane waves and $q$ and $q'$ are
the wavevectors of the scattered waves. The symbol $\langle \rangle$ denotes the average over a
set of surface profiles. $I(q|k)$ is the intensity of the scattered light. We shall study
this correlator in a multiple scattering treatment which yields $C^{(1)}$, $C^{(2)}$ and $C^{(3)}$
correlators as well as new $C^{(10)}$ and $C^{(1.5)}$ correlators which have not previously
been treated in the literature for either surface or volume scattering.

The best known angular correlation effects are the memory effect and time-
reversed memory effect in $C^{(1)}$. These effects give correlations, $C^{(1)}$, which are
non-zero only when $k - k' = q - q'$. This is the lowest order effect that has
been predicted and observed in many works on surface and volume scattering of
light. In this dissertation we predict a new low-order correlation, $C^{(10)}$, that is
non-zero only when $q + q' = k + k'$ and has not been previously studied. We also
predict several other high-order correlators $C^{(1.5)}$, $C^{(2)}$, $C^{(3)}$ which are related to
the surface electromagnetic waves — surface polaritons. It should be noted that
these high order correlators are not restricted to the specific values of $k$, $k'$, $q$ and
$q'$ as are the $C^{(1)}$ and $C^{(10)}$ correlators. These higher order correlators exhibit
novel peaks when studied as functions of $k$, $k'$, $q$ and $q'$ which allow us to obtain
information about surface electromagnetic waves from the speckle pattern. In the Section V.2, we start with a discussion about the perturbation theory we used to obtain the scattered electromagnetic field and how we use these results to compute the correlator (V.2). Next in the Section V.3, we present the results for the speckle correlators, obtained from the perturbation theory. Then, in the Section V.4, we present the results for the speckle correlations obtained by direct numerical generation of random surfaces, calculation of field and direct configuration averaging the field products expressing the correlators. These results give very similar results to those in the section V.3.

V.2. Perturbation Theory for Light Scattering From the 1D Randomly Rough Metal Surface

We study the following problem: An electromagnetic plane wave with the wavevector component \( k \) parallel to the mean scattering surface is incident on a randomly rough metal surface Figure 19. The scattered light is a superposition of plane waves with the different wavevectors component \( q \) parallel to the mean surface.

The one field component of the electromagnetic wave is taken to be of the form \( A = (0, A_2, 0) \) such that:

\[
A_2^s = \exp(ikx_1 - i\alpha_0(k, \omega)x_3) + \int \frac{dq}{2\pi} R(q|k) \exp(iqx_1 + i\alpha_0(q, \omega)x_3) \quad (V.3a)
\]

\[
A_2^p = \int \frac{dq}{2\pi} A(q, k) \exp(iqx_1 - i\alpha_1(q, \omega)x_3) \quad (V.3b)
\]

where \( A = E \) for \( s \) polarization and \( = H \) for \( p \) polarization. The other components of the electromagnetic field are obtained from Eq. (V.3) by using Maxwell's
equations. Because of the symmetry of our system in the \( x_2 \) direction there is no mixing between \( s \) and \( p \) polarizations and there is no cross-polarization term in the (V.3).

In this section, we will study \( p \)-polarization only because only \( p \) polarization excites surface electromagnetic waves. \( s \)-polarization does not produce such excitations. The scattering amplitude \( R(q|k) \) can be determined from the electromagnetic boundary conditions. Doing this we find that the scattering amplitude is proportional to the Green's function, \( G(q|k) \), for surface polaritons of the rough surface. So that

\[
R(q|k) = -iG(q|k)(2\alpha(k,\omega))
\]  

This Green's function satisfies Dyson's equation

\[
G(q|k) = 2\pi\delta(q - k)G_0(k) + G_0(q) \int \frac{dp}{2\pi} V(q|p)G(p|k)
\]

with the interaction \( V(q|p) \), where \( V(q|p) \) represents the scattering of the surface polaritons by the surface roughness and

\[
G_0(k) = \frac{i\varepsilon(\omega)}{\varepsilon(\omega)\alpha_0(k,\omega) + \alpha(k,\omega)}
\]

is the Surface polariton Green's function for a flat metal surface. The interaction, \( V(q|p) \) is non–zero when we have a rough surface and for weakly rough surfaces can be taken in the form:

\[
V(q|k) = [(\varepsilon - 1)/\varepsilon^2](\varepsilon qk - \alpha(q,\omega)\alpha(k,\omega))\zeta(q - k)
\]
The Dyson's equation (V.5) can be represented in the following diagrammatic form:

\[
\begin{array}{c}
\uparrow \\
- \\
\downarrow \\
\end{array}
\]

(V.8)

The Dyson's equation (V.5), (V.8) is an equation for the single-particle Green's function \( G(q|k) \). The differential reflection coefficient we studied in the Chapter IV is proportional to the average of 2-particle Green's function \( \langle G(q|k)G^*(q'|k') \rangle \). Specifically the incoherent scattering is given by:

\[
\left\langle \frac{\partial R}{\partial \theta_s} \right\rangle_{\text{incoh}} = \frac{1}{L} \omega^2 \pi \cos^2 \theta_s \cos \theta_i \left\{ \langle |G(q|k)|^2 \rangle - \langle |G(q|k)| \rangle^2 \right\}
\]

(V.9)

In the correlator (V.2) the intensity \( I(q|k) \) is defined by

\[
I(q|k) = \frac{\omega}{c} \frac{\alpha_0(q, \omega)}{\alpha_0(k, \omega)} |R(q|k)|^2
\]

(V.10)

The correlator (V.2) is proportional to the average of 4-particle Green's function

\[
C(q, k|q', k') = \frac{1}{L^2} \frac{\omega^4}{c^4} 16 \cos \theta_i \cos \theta_s \cos \theta'_i \cos \theta'_s \left\{ \langle |G(q|k)|^2 \rangle \langle |G(q'|k')|^2 \rangle - \langle |G(q|k)| \rangle^2 \langle |G(q'|k')|^2 \rangle \right\}
\]

(V.11)

Now the problem of the calculation of the speckle correlator \( C(q, k|q', k') \) is the problem of calculating average \( \langle |G(q|k)|^2|G(q'|k')|^2 \rangle \). This average can be calcu-
lated numerically (see Section V.4) or by applying a perturbation theory. In this section we will discuss the perturbation theory.

The perturbation theory that we applied to the calculation of (V.11) is based on the assumption that our surface profile function satisfies Gaussian statistics. For Gaussian statistics of $\zeta(x_1)$ the value of $\langle \zeta^n(x_1)\zeta^m(x_2) \rangle$ can be expressed through low order moments defined in (V.1) by applying Price's theorem [24]. Application of this theorem to perturbation theory terms allows us to express all the contributions to $C(q,k|q',k')$ from Eq. (V.11) in terms of $\langle G^*(q|k)G(q'|k') \rangle$ and $\langle G(q|k)G(q'|k') \rangle$.

The two–particle Green's function $\langle G^*(q|k)G(q'|k') \rangle$ is the solution of the Bethe–Salpeter equation

$$\langle G^*(q|k)G(q'|k') \rangle = 2\pi \delta(q - k)2\pi \delta(q' - k')G^*(k,\omega)G(k',\omega)$$

$$+ G^*(q,\omega)G(q',\omega) \int \frac{dr}{2\pi} \int \frac{ds}{2\pi} \langle \Gamma(q,r|q',s) \rangle \langle G^*(r|k)G(s|k') \rangle,$$  \hspace{1cm} (V.12)

where $\langle \Gamma(q,r|q',s) \rangle$ is the irreducible vertex function, and $2\pi \delta(q - k)G(k,\omega) = \langle G(q|k) \rangle$. For weakly rough surfaces we use Eq. (V.7) and the pole approximation to compute $\langle \Gamma(q,r|q',s) \rangle$ in the ladder and maximally crossed diagram approximation (see Ref. [37] for details). In the pole approximation we have

$$G(k,\omega) \cong C_1 \left\{ \frac{1}{k - K_{sp} - i\Delta_{tot}} - \frac{1}{k + K_{sp} + i\Delta_{tot}} \right\},$$  \hspace{1cm} (V.13)

where

$$C_1 = \frac{\epsilon_1(\omega)\sqrt{-\epsilon_1(\omega)}}{1 - \epsilon_1^2(\omega)}$$  \hspace{1cm} (V.14a)

$$\Delta_{tot} = \Delta_\epsilon + \Delta_{sp}$$  \hspace{1cm} (V.14b)
\[ \Delta_t = \frac{\epsilon_2(\omega)K_{sp}}{2\epsilon_1(\omega)[\epsilon_1(\omega) + 1]} \]  
\[ \Delta_{sp} = 2C_1^2\sigma^2 \left[ \frac{\epsilon_1(\omega) - 1}{\epsilon_1(\omega)} \right]^2 K_{sp}^2 g(2K_{sp}) \]  
\[ K_{sp} = \frac{\omega}{c} \sqrt{\frac{\epsilon_1(\omega)}{\epsilon_1(\omega) + 1}}. \]

\(K_{sp}\) defined in Eq. (V.14e) is the wavenumber of the surface plasmon polariton of frequency \(\omega\) at the planar vacuum-metal interface, and \(\Delta_{tot}\) given by Eqs. (V.14) is the reciprocal of the amplitude mean free path of the surface plasmon polaritons at the vacuum-metal interface.

Employing this approximation we find

\[
\langle G^\ast(q|k)G(q'|k') \rangle = 2\pi \delta(q - k)2\pi \delta(q' - k')G^\ast(k, \omega)G(k', \omega) + 2\pi \delta(q - k - q' + k')G^\ast(q, \omega)G(q', \omega)G(k, \omega)G(k', \omega)\mathcal{L}(q, k|q', k'), \tag{V.15}
\]

where

\[
\mathcal{L}(q, k|q', k') = V_0(q, k|q', k') + 2C_1^2\frac{\Delta_{tot}}{1 - \frac{\Delta_{sp}}{\Delta_{tot}}} \left\{ \frac{1}{(k - k')^2 + 4\Delta_{tot}^2} \right\} \]

\[
\times \left[ V_0(q, K_{sp}|q', K_{sp})V_0(K_{sp}, k|K_{sp}, k') + V_0(q, -K_{sp}|q', -K_{sp})V_0(-K_{sp}, k| - K_{sp}, k') \right. 
\]

\[
+ \frac{\Delta_{sp}}{\Delta_{tot}} \left( V_0(q, K_{sp}|q', K_{sp})V_0(-K_{sp}, k| - K_{sp}, k') + V_0(q, -K_{sp}|q', -K_{sp})V_0(K_{sp}, k|K_{sp}, k') \right) \]

\[
+ \frac{1}{(q + k')^2 + 4\Delta_{tot}^2} \left[ V_0(q, K_{sp}| - K_{sp}, k')V_0(K_{sp}, k|q', -K_{sp}) + V_0(q, -K_{sp}|K_{sp}, k')V_0(-K_{sp}, k|q', K_{sp}) + \frac{\Delta_{sp}}{\Delta_{tot}} \left( V_0(q, K_{sp}| - K_{sp}, k')V_0(-K_{sp}, k|q', K_{sp}) \right) \right] \]

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\[ + V_0(q, -K_{sp}|K_{sp}, k') V_0(K_{sp}, k|q', -K_{sp}) \} \right) \], \quad (V.16) \]

and

\[
V_0(q, r|s, t) = \sigma^2 g(|q - r|) \left| \frac{\epsilon(\omega) - 1}{\epsilon^2(\omega)} \right|^2 \\
\times [\epsilon(\omega)qr - \alpha(q, \omega)\alpha(r, \omega)]^* \\
\times [\epsilon(\omega)st - \alpha(s, \omega)\alpha(t, \omega)] \quad (V.17)
\]

and the \( G \)'s multiplying \( \mathcal{L} \) on the right hand side of Eq. (V.15) can be approximated as in Ref. [37] by \( G_0 \)'s.

In Eq. (V.16) we have retained terms of higher order in the perturbation theory in \( \zeta(x_1) \) than just the \( \zeta^2(x_1) \) terms in \( \langle G^*(q|k)G(q'|k') \rangle \), as these represent important phase coherent processes which give rise to the \( 1/[(k - k')^2 + 4\Delta_{\text{tot}}^2] \) and \( 1/[(q + k')^2 + 4\Delta_{\text{tot}}^2] \) factors in the two-particle Green's function. The factor containing \( k - k' \) arises from the ladder diagrams, and the factor containing \( q + k' \) arises from the maximally-crossed diagrams, which represent the time-reversed phase coherent effects that are known as weak localization. These two factors give rise to important features in \( C(q, k|q', k') \).

The two-particle Green's function \( \langle G(q|k)G(q'|k') \rangle \), computed from the ladder and maximally crossed diagrams, does not exhibit significant features such as the factors containing \( k - k' \) and \( q + k' \) found in Eq (V.16). Instead it is a slowly varying function of \( q, k, q' \) and \( k' \). Consequently, in the small roughness approximation we take

\[
\langle G(q|k)G(q'|k') \rangle \cong 2\pi \delta(q - k + q' - k') G_0(q, \omega)G_0(q', \omega) \\
\times G_0(k, \omega)G_0(k', \omega) U(q, k|q', k'), \quad (V.18)
\]
where

\[
(\mathcal{V}(q|k)\mathcal{V}(q'|k')) = 2\pi\delta(q - k + q' - k')U(q, k|q', k'),
\]  \hspace{1cm} (V.19)

with

\[
U(q, k|q', k') = \sigma^2 g(|q - k|) \left[ \frac{\epsilon(\omega) - 1}{\epsilon^2(\omega)} \right]^2 \times [\epsilon(\omega)qk - \alpha(q, \omega)\alpha(k, \omega)] \times [\epsilon(\omega)q'k' - \alpha(q', \omega)\alpha(k', \omega)].
\]  \hspace{1cm} (V.20)

For easy writing of perturbation terms to (V.11) it is very convenient to represent \( G_0(k), \mathcal{L}(q, k|q', k') \) and \( U(q, k|q', k') \) calculated above in the diagrammatic form. The definitions are shown in Figure 20.

Figure 20. Definitions of the Diagrammatic Representations for the Green’s Functions and the Four-Vertex Terms Which Enter Into The Diagrammatic Representation of \( G_0(q) \) and Four-Vertexes \( \mathcal{L}(q, k|q', k') \) and \( U(q, k|q', k') \) From Eqs. (V.6), (V.16) and (V.20).
V.2.1. $C^{(1)}$ Memory Effect and $C^{(10)}$ Term

The lower order contributions to the $\langle |G(q|k)|^2|G(q'|k')|^2 \rangle$ can be obtained by applying the approximation

$$\langle |G(q|k)|^2|G(q'|k')|^2 \rangle \cong \langle |G(q|k)|^2 \rangle \langle |G(q'|k')|^2 \rangle$$

$$+ \langle G^*(q|k)G(q'|k') \rangle \langle G^*(q'|k')G(q|k) \rangle$$

$$+ \langle G^*(q|k)G^*(q'|k') \rangle \langle G(q'|k')G(q|k) \rangle.$$  \hspace{1cm} (V.21)

It should be pointed out here, that the factorization approximation [53], used in previous studies of speckle correlations in the scattering of light from disordered media, and which is valid for a circular complex Gaussian random process, consists in keeping only the second term on the right-hand side of Eq. (V.21). In what follows we do not employ the factorization approximation.

The first term on the right-hand side of Eq. (V.21) is a specular term and is non-zero only for $q = k$ and $q' = k'$. The second term is non-zero for $q - k - q' + k'$ and describes the well-known memory and time-reversed memory effects. The third term is non-zero for $q - k + q' - k'$ and describes the $C^{(10)}$ correlations. The corresponding contributions to the speckle correlator (V.11) can be represented in diagrammatic form shown in Figure 21. The diagrammatic contributions in Figure 21 can be easily translated to formulae by using definitions in Figure 20.
V.2.2. $C^{(1.6)}$ Surface Plasmon Polariton Effects

In the next higher order in $\zeta(x_1)$ (order $\zeta^6(x_1)$) in the diagrammatic contributions to $C(q, k|q', k')$ which exhibit peaks related to the propagation of surface plasmon polaritons along the vacuum-metal interface. In addition, in this order the wavenumbers $q, k, q', k'$ are no longer constrained by the factors $2\pi \delta(q - k - q' + k')$ or $2\pi \delta(q - k + q' - k')$ present in the contributions to $C(q, k|q', k')$ described in Eq. (V.11).

In Figures 22a through 22h we list the diagrammatic contributions to $C(q, k|q', k')$ of order $\zeta^6(x_1)$ which produce peaks when $q - q' + k' = \pm K_{sp}$, $k - k' + q' = \pm K_{sp}$, $q' - q + k = \pm K_{sp}$, $q - k + k' = \pm K_{sp}$, $q + q' - k' = \pm K_{sp}$, $k + k' - q = \pm K_{sp}$, $q + q' - k = \pm K_{sp}$, $q + q' - k = \pm K_{sp}$, respectively. Other diagrams which we have not listed can give rise to peaks provided that two of the four $q, q', k, k'$ are equal. We have not considered these cases here.

V.2.3. $C^{(2)}$ Terms of Order $\zeta^8(x_1)$

In the next higher order in $\zeta(x_1)$ (order $\zeta^8(x_1)$) in the diagrammatic contributions to $C(q, k|q', k')$ which exhibit peaks at $q' = \pm k'$, $\pm k, \pm q$. These peaks
Figure 22. Diagrams Which Contribute the Most Dominant Peaks in the $C^{(1,5)}(q, k|q', k')$ Contribution to $C(q, k|q', k')$. 

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are again associated with surface plasmon polariton poles in the Green's function. As with $C^{(1-5)}$, the $C^{(2)}$ contributions are no longer constrained by factors such as $2\pi \delta(q - k - q' + k')$ or $2\pi \delta(q - k + q' - k')$, but exhibit a general dependence on $q, k, q', k'$.

In Figures 23a through 23n we present the diagrams in $D(q, k|q', k')$ of order 8 which give rise to peaks in the correlation function $C(q, k|q', k')$ when $q' = k'$, $q' = q$, $k' = -q$, $q' = -k$, $k' = k$, $q = k$, $k' = q$, $q' = -q$, $k' = -k$, respectively.

V.3. Speckle Correlation From One-Dimensional Randomly Rough Surfaces: Results

We have evaluated the results for $C(q, k|q', k')$ described above for light whose wavelength is 4579Å incident on a silver surface for which $\epsilon(\omega) = -7.5 + i0.24$. We have considered a Gaussian random surface with $W(|x_1|) = \exp(-x_1^2/a^2)$ for $a = 1000\,\text{Å}$ and $\sigma = 50\,\text{Å}$.

In Figure 24 we present results for $C^{(1)}(q, k|q', k')$ and $C^{(10)}(q, k|q', k')$ versus $\theta'_s$ for $\theta_s = -10^\circ$ and $\theta_i = 20^\circ$. Note that in the case of $C^{(1)}$, once $q$, $k$ and $q'$ are specified $k'$ is obtained from the relation $q - k - q' + k' = 0$. Two peaks are observed in $C^{(1)}$ as a function of $\theta'_s$, one at $q' = q$ ($\theta'_s = \theta_s$) and another at $q' = -k$ ($\theta'_s = -\theta_i$). These peaks arise from phase coherent effects associated with the resonant excitation of surface polaritons, and their full width at half maximum is $4\Delta_{\text{tot}}$. In the case of $C^{(10)}$, once $q$, $k$ and $q'$ are specified, $k'$ is obtained from the relation $q - k + q' - k' = 0$. In this case no peaks are observed in $C^{(10)}$ as a function of $\theta'_s$, but $C^{(10)}$ is a slowly varying function of $\theta'_s$ over the region for which $q - k + q' - k' = 0$.
Figure 23. Diagrams Which Contribute the Most Dominant Peaks in the $C^{(2)}(q, k|q', k')$ Contribution to $C(q, k|q', k')$. 

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Figure 24. Plots of $C^{(1)}(q, k|q', k')$ (Solid Line) and $C^{(10)}(q, k|q', k')$ (Dashed Line) Versus $\theta_s'$ for the One-Dimensional Random Rough Surface.

In Figure 25 we present results for $C^{(1.5)}(q, k|q', k')$ versus $\theta_s'$ for $\theta_s = -10^\circ$, $\theta_i = 20^\circ$, and $\theta_i' = 30^\circ$. In this case $q'$ is not restricted by the values of $q, k, k'$, but ranges freely over the interval $-\omega/c < q' < \omega/c$. A number of peaks are observed in this correlation function. These occur for a number of cases in which a linear combination of three of the wavenumbers $q, k, q', k'$ add to $\pm K_{sp}$. These specific combinations and the values of $\theta_s'$ at which they give rise to peaks in $C^{(1.5)}$ are shown in Table 2.

In Figure 26 we present results for $C^{(2)}(q, k|q', k')$ versus $\theta_s'$ for $\theta_s = -10^\circ$, $\theta_i = 20^\circ$ and $\theta_i' = 30^\circ$. In this case $q'$ is not restricted by the values of $q, k, k'$, but ranges freely over the interval $-\omega/c < q' < \omega/c$. Several peaks are observed in this figure. These occur for a number of cases in which a linear combination of two of the wavenumbers $q, k, q', k'$ add to zero. These specific combinations and the values of $\theta_s'$ at which they give rise to peaks in $C^{(2)}$ are shown in Table 2.

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V.4. Numerical Simulations of Speckle Correlation

A drawback of diagrammatic perturbation theory results is that one must be careful to choose the most important diagrams which contribute to the quantity which is being computed. This is not always easy to do and, in general, not all possible diagrammatic contributions can be included in such a computation. To re-enforce the results of our diagrammatic methods presented above we now present the results of some computer simulation calculations of $C^{(1)}, C^{(10)}, C^{(1.5)}$ and $C^{(2)}$ for one dimensional randomly rough surfaces.

Specifically, we simulate these correlators as follows. A Monte Carlo routine is used to generate a set of Gaussian random surfaces which exhibit the statistical properties of the surfaces used in the perturbation calculations above. The scattering of an incident plane wave is computed for each of the random surfaces.
Table 2

Peaks in $C^{(1.5)}(q, k|q', k')$ and $C^{(3)}(q, k|q', k')$ for the One-Dimensional Rough Surface

<table>
<thead>
<tr>
<th>$\theta'$</th>
<th>Peak Condition</th>
<th>Correlation Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>-66.4°</td>
<td>$-k' + k + q' = -K_{sp}$</td>
<td>$C^{(1.5)}$</td>
</tr>
<tr>
<td>-48.4°</td>
<td>$q - q' + k' = K_{sp}$</td>
<td>$C^{(1.5)}$</td>
</tr>
<tr>
<td>-34.0°</td>
<td>$q' + q - k = -K_{sp}$</td>
<td>$C^{(1.5)}$</td>
</tr>
<tr>
<td>-23.6°</td>
<td>$q' - k' + q = -K_{sp}$</td>
<td>$C^{(1.5)}$</td>
</tr>
<tr>
<td>-13.4°</td>
<td>$k + k' - q' = K_{sp}$</td>
<td>$C^{(1.5)}$</td>
</tr>
<tr>
<td>34.0°</td>
<td>$q' - q + k = K_{sp}$</td>
<td>$C^{(1.5)}$</td>
</tr>
<tr>
<td>-20.0°</td>
<td>$q' = -k$</td>
<td>$C^{(2)}$</td>
</tr>
<tr>
<td>-10.0°</td>
<td>$q' = q$</td>
<td>$C^{(2)}$</td>
</tr>
<tr>
<td>10.0°</td>
<td>$q' = -q$</td>
<td>$C^{(2)}$</td>
</tr>
<tr>
<td>20.0°</td>
<td>$q' = k$</td>
<td>$C^{(2)}$</td>
</tr>
</tbody>
</table>

generated. For $p$– polarized waves we used Maradudin and Méndez [35] theory for the scattering of electromagnetic waves from weakly randomly rough surfaces (see Appendix A for brief description of how the scattered electromagnetic fields are related to surface profile using the Maradudin and Méndez theory). This theory expresses the scattered field above a one–dimensional random rough surface in a perturbation expansion which is correct to third order in $\zeta(x_1)$ and does not involve a pole approximation. In the present calculations we retain only the terms through second order in this expansion. For $s$– polarized wave we extended the
Figure 26. Plots of $C^{(2)}(q, k|q', k')$ Versus $\theta'_s$ for the One-Dimensional Random Rough Surface.

Maradudin and Méndez theory to the case of $s-$polarization (see Appendix B).

We shall now give a brief description of how the random surfaces that were used to compute the correlations from the Maradudin and Méndez theory were generated. This will be followed by a presentation of results from this simulation.

V.4.1. The Random Surfaces Generation

To generate a random surface with the statistical properties of (V.1) we used the method in Ref. [34]. Specifically, the surface profile function $\zeta(x_1)$ can be written as the Fourier transform.

$$\zeta(x_1) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \zeta(k) \exp(ikx_1) . \quad (V.22)$$

Substituting (V.22) into (V.1), we can find that $\zeta(k)$ obeys the following statistical
relations:

\[ \langle \zeta(k) \rangle = 0 \quad (V.23a) \]
\[ \langle \zeta(k) \zeta^*(k') \rangle = 2\pi \delta(k - k')g(|k|) \quad (V.23b) \]

For the computer simulation we need to replace all the integrals in equations below by sums. Specifically, we performed a discretization of \( k \) so that \( k \) can take only values of

\[ k = nk_{\text{step}}, \quad n = \{-N, \ldots, -2, -1, 0, 1, 2, \ldots, N\} \quad (V.24) \]

where \( k_{\text{step}} \) is a small value to be given below. Then all the integrals can be replaced by sums as:

\[ +\int_{-\infty}^{\infty} \frac{dk}{2\pi} f(k) \approx \frac{k_{\text{step}}}{2\pi} \sum_{n=-N}^{n=N} f(nk_{\text{step}}) \quad (V.25) \]

Following Ref. [34], we take the expression for \( \zeta(k) \) to be of the form:

\[ \zeta(nk_{\text{step}}) = \sqrt{\frac{2\pi}{k_{\text{step}}}} \frac{X_n + iY_n}{\sqrt{2}} \sqrt{g(nk_{\text{step}})} \quad (V.26) \]

where \( X_n \) and \( Y_n \) (\( n = -N \ldots N \)) are independent Gaussian random numbers of zero mean and a dispersion equal to one. A direct check shows that when we use (V.25) the approximation for \( \zeta(k) \) from Eq. (V.26) satisfies Eqs. (V.1), (V.23), and the relation between high- and low- order moments for random process \( \zeta(x_1) \) is the same as it is for a Gaussian random process.
V.4.2. Numerical Simulation. Results

In Figure 27 we present results for the computer simulation generated correlators plotted versus $\theta'$ which were computed using the Maradudin and Méndez theory [35]. The results presented are for comparison with the perturbation theory results in Figures 24 through 26 above. In obtaining the results 100,000 random surface profiles were used to compute the correlator averages. The following $N$ and $k_{\text{step}}$ were taken in (V.24): $N = 700$ and $k_{\text{step}} = 5.2/(aN)$. The values of $\lambda$, $\sigma$, $a$, and $\epsilon(\omega)$ used in the simulation were the same as those used in plotting Figures 24 through 26. The results for $C^{(1)}$ and $C^{(10)}$ were obtained by retaining the terms of order $\zeta^4(x_1)$. The $C^{(1.5)}$ results were obtained by retaining the terms of order $\zeta^6(x_1)$. The $C^{(2)}$ results were obtained by retaining the terms of order $\zeta^8(x_1)$.

In general, good agreement is found between the results obtained using perturbation theory and the simulation method in the two different formulations. This gives us confidence in our choice of the diagrams we have used in the perturbation calculations we have presented in Sections V.2 and V.3.

A second set of simulation results are presented in Figure 28. These are for the scattering of $s$-polarized light from the one-dimensional surface studied in obtaining Figures 24 through 26. They were obtained using the theory from appendix B for $s$-polarization and the simulations for this case where made using 10,000 random surface profiles and the following $N$ and $k_{\text{step}}$ were taken in (V.24): $N = 700$ and $k_{\text{step}} = 5.2/(aN)$. Otherwise the simulation was run as in the case that led to the results presented in Figure 27. Aside from some peaks associated with coherent scattering there are no peaks present in the plots of $C^{(1.5)}$ and $C^{(2)}$. 

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Figure 27. Computer Simulation Results Based on the Maradudin and Méndez Theory for the Scattering of \( p \)-polarized Light From a One-Dimensional Randomly Rough Surface. (a) \( C^{(1)}(q, k|q', k') \) (Solid Line) and \( C^{(10)}(q, k|q', k') \) (dashed line) Versus \( \theta' \); (b) \( C^{(1.5)}(q, k|q', k') \) Versus \( \theta' \); and (c) \( C^{(2)}(q, k|q', k') \) Versus \( \theta' \).
Figure 28. Same as in Figure 27 But Now for the Scattering of $s$– Polarized Light.
These indicate the absence of surface plasmon polariton effects for the weakly rough surface for $s$—polarization scattering. This is not surprising, because it is known that the only surface plasmon polaritons that can exist on a weakly rough surface are $p$—polarized, and they can be excited only by $p$—polarized light in scattering from a one—dimensional surface.
CHAPTER VI

CONCLUSION

We have studied four projects in this dissertation:

1. Thermal conductivity study of amorphous insulating solids (Chapter II).

2. Localization in a one-dimensional optical system (Chapter III).

3. Determination of the surface profile statistics from the optical scattering data (Chapter IV).

4. Speckle correlation study of light multiply scattered from the randomly rough metal surfaces (Chapter V).

In the first project we have computed the thermal conductivity of a model composed of a fcc percolating cluster of atoms. Unlike previous treatments we have allowed the atoms in the system to undergo full three-dimensional motion. Our model exhibits three experimental observed region of temperature behavior ($T^\beta$ region, plateau region and monotonic increase region). The exponent $\beta$ in our model satisfies $1 \leq \beta \leq 2$ which is more realistic than $\beta = 2$ observed in the previous scalar wave treatments of this problem. The origin of this difference is in the density of states that in 3D treatment exhibit a depart from Debye density of states. These results are published in Ref. [30].

In the second project we have studied Anderson localization in 1D system that consists of a semi-infinite array of variable alternating layers of dielectric separated by vacuum layers which have electromagnetic waves incident on them.
slabs are random values. Strong polarization dependence of the localization length is obtained. The results are obtained for plane wave and Gaussian beam incident to the system. The \( p \) polarization of a beam has a strong dependence of the localization length on the beam's width because of Brewster's angle anomaly (infinite localization length for \( p \)-polarized plane wave incident at Brewster's angle). Preliminary results for 2D system are also obtained.

In the third project we applied the Reverse Monte Carlo technique for the determination of surface profile statistics from the optical scattering data. The Reverse Monte Carlo technique has recently been developed and applied to the determination of the structures of amorphous and polymer materials from X-ray scattering data. We have studied a 1D randomly rough metal surface and used Reverse Monte Carlo method for the determination of the surface profile statistics from measured differential reflection data for the scattering of electromagnetic radiation. First the RMC employs Monte Carlo techniques for random generation of surface statistics. Then the Differential Reflection Coefficient that describes the angular distribution of the scattered field for these simulated surface statistical properties, is calculated by applying a perturbation theory. Next the RMC employs a maximal entropy approach that allows for the determination from the generated surface statistics of those statistics that best fit the experimental data. Excellent agreement with the power spectrum data obtained from contact profilometry methods is observed. These results are published in Ref. [31].

In the fourth project we studied the speckle correlations in the scattered light. When an incident light scatters from a randomly rough surface we obtain speckle structure in the intensity of scattered light. The correlation in the intensity between different speckle patterns is a subject of study in the fourth project. Along
with well known memory and reverse-memory effect, denoted as $C^{(1)}$, that were observed in the bulk materials several new correlations have being found. We predict a new low-order correlation, $C^{(10)}$, that is non-zero only when $q + q' = k + k'$ and has the same order as $C^{(1)}$. We also predict several other high-order correlators $C^{(1.5)}, C^{(2)}, C^{(3)}$ which are related to the surface electromagnetic waves — surface polaritons. It should be noted that these high order correlators are not restricted to the specific values of $k$, $k'$, $q$ and $q'$ as are $C^{(1)}$ and $C^{(10)}$. These high order correlators exhibit novel peaks which allow us to obtain information about surface electromagnetic waves from the speckle pattern. The results we obtained both by applying a perturbation theory and by numerical simulations. These results are published in Refs. [32,33]
Appendix A
Second Order Scattering Amplitude for $p$-Polarization
In this appendix we express the scattering amplitude from (V.3) for \( p \) polarization via Fourier transform of surface profile \( \zeta(k) \). For \( p \) polarization \( A = H \) in (V.3))

We start with the boundary conditions on the interface \( x_3 = \zeta(x_1) \):

1. \( H_2 \) is continuous at \( x_3 = \zeta(x_1) \).
2. \( E_\tau \) is continuous at \( x_3 = \zeta(x_1) \).

Where

\[
\tau = \frac{1}{\sqrt{1 + \zeta^2}} [1, 0, \zeta'] \quad (A.1)
\]

Then the boundary conditions can be written in the form:

\[
\begin{align*}
\left( H_2^\zeta - H_2^e \right) & \bigg|_{x_3 = \zeta(x_1)} = 0 \quad (A.2) \\
\left( E_1^\zeta + \zeta' E_3^\zeta - E_1^e - \zeta' E_3^e \right) & \bigg|_{x_3 = \zeta(x_1)} = 0 \quad (A.3)
\end{align*}
\]

(The factor \( \sqrt{1 + \zeta'^2} \) cancels in the left and right hand side of the Eq.(A.3)).

Substituting

\[
\begin{align*}
E_3 &= \frac{ic \, \partial H_2}{\omega \epsilon \partial x_1} \quad (A.4a) \\
E_1 &= -\frac{ic \, \partial H_2}{\omega \epsilon \partial x_3} \quad (A.4b)
\end{align*}
\]

into (A.3) we obtain:

\[
\begin{align*}
\left( H_2^\zeta - H_2^e \right) & \bigg|_{x_3 = \zeta(x_1)} = 0 \quad (A.5a) \\
\left( - \frac{\partial H_2^\zeta}{\partial x_3} + \zeta' \frac{\partial H_2^e}{\partial x_1} + \frac{1}{\epsilon} \frac{\partial H_2^e}{\partial x_3} - \zeta' \frac{\partial H_2^e}{\partial x_1} \right) & \bigg|_{x_3 = \zeta(x_1)} = 0 \quad (A.5b)
\end{align*}
\]

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Now let us take $H_2$ in the form

$$H_2^e = \exp(ikx_1 - i\alpha_0(k)x_3) + \int \frac{dq}{2\pi} R(q, k) \exp(iqx_1 + i\alpha_0(q)x_3)$$  \hspace{1cm} (A.6a)$$

$$H_2^\delta = \int \frac{dq}{2\pi} A(q, k) \exp(iqx_1 - i\alpha_1(q)x_3)$$  \hspace{1cm} (A.6b)

We treat this problem using second order perturbation theory:

$$R(p, k) = 2\pi \delta(p - k)R_0(k) + R_1(p, k)\zeta(p - k) + R_2(p, k)$$ \hspace{1cm} (A.7a)

$$A(p, k) = 2\pi \delta(p - k)A_0(k) + A_1(p, k)\zeta(p - k) + A_2(p, k)$$ \hspace{1cm} (A.7b)

Substituting (A.7) into the boundary conditions (A.2) and (A.3) combining all terms up to the second order together we obtain:

$$R_0(k) = \frac{\alpha_0(k) - \alpha_1(k)}{\alpha_0(k) + \frac{\alpha_1(k)}{\epsilon}}$$  \hspace{1cm} (A.8a)$$

$$A_0(k) = \frac{2\alpha_0(k)}{\alpha_0(k) + \frac{\alpha_1(k)}{\epsilon}}$$  \hspace{1cm} (A.8b)

The matrix $M(p)$ is defined as follows:

$$M(p) = \frac{1}{\alpha_0(p) + \frac{\alpha_1(p)}{\epsilon}} \begin{pmatrix} \frac{\alpha_1(p)}{\epsilon} & -1 \\ -\alpha_0(p) & -1 \end{pmatrix}$$ \hspace{1cm} (A.9)

The values $V_1(p, k)$ and $V_2(p, k)$ and $X_j(p, k)$ are defined as follows:

$$X_j(p, k) = \begin{pmatrix} R_j(p, k) \\ A_j(p, k) \end{pmatrix}$$ \hspace{1cm} (A.10)
\[ V_1(p, k) = i \left( \frac{1}{\varepsilon} - 1 \right) A_0(k) \left( \begin{array}{c} \alpha_1(k) \\ k_p \end{array} \right) \] (A.11)

\[ V_2(p, k) = \left( \begin{array}{c} \int \frac{dq}{2\pi} \zeta(p-q)\zeta(q-k)g_R(q, p, k) \\ \int \frac{dq}{2\pi} \zeta(p-q)\zeta(q-k)g_A(q, p, k) \end{array} \right) \] (A.12)

where

\[ g_R(q, p, k) = \frac{1 - \varepsilon}{2} A_0(k) \frac{\omega^2}{c^2} - i\left\{ \alpha_0(q) R_1(q, k) + \alpha_1(q) A_1(q, k) \right\} \] (A.13)

\[ g_A(q, p, k) = \alpha_1(k) \frac{1 - \varepsilon}{2\varepsilon} A_0(k) \frac{\omega^2}{c^2} + i \left\{ \frac{\omega^2}{c^2} - qp \right\} R_1(q, k) - \left[ \frac{\omega^2}{c^2} - \frac{qp}{\varepsilon} \right] A_1(q, k) \] (A.14)

Then \( X_1 \) and \( X_2 \) can be calculated as follows \( (j = 1, 2) \):

\[ X_j(p, k) = M(p)V_j(p, k) \] (A.15)

And the answer is:

\[ \begin{pmatrix} R(p, k) \\ A(p, k) \end{pmatrix} = 2\pi \delta(p - k) \begin{pmatrix} R_0(k) \\ A_0(k) \end{pmatrix} + M(p) \times (\zeta(p - k)V_1(p, k) + V_2(p, k)) \] (A.16)
Appendix B
Second Order Scattering Amplitude for $s$-Polarization
In this appendix we present an expression for the scattering amplitude from (V.3) for s polarization (in this case \( A = E \) in (V.3)) via Fourier transform of surface profile \( \zeta(k) \). For the s polarization we have the same boundary conditions as we have for p polarization in (A.2) and (A.3). There is only a difference that here we use the electric field \( E = (0, E_2, 0) \) instead of magnetic field in Appendix A

\[
E_2^\zeta = \exp(ikx_1 - i\alpha_0(k)x_3) + \int \frac{dq}{2\pi} R(q, k) \exp(iqx_1 + i\alpha_0(q)x_3) \quad \text{(B.1a)}
\]
\[
E_2^\zeta = \int \frac{dq}{2\pi} A(q, k) \exp(iqx_1 - i\alpha_1(q)x_3) \quad \text{(B.1b)}
\]

The expression for \( R(q, k) \) in the case of s polarization is given by formulaes (A.11), (A.12) and (A.16) where

\[
R_0(k) = \frac{\alpha_0(k) - \alpha_1(k)}{\alpha_0(k) + \alpha_1(k)} \quad \text{(B.2a)}
\]
\[
A_0(k) = 1 + R_0(k) \quad \text{(B.2b)}
\]

\[
V_1(p, k) = i\frac{\omega^2}{c^2} A_0(k)(1 - \epsilon) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{(B.3)}
\]

and \( g_R(q, p, k) \) and \( g_A(q, p, k) \) in (A.12) now are equal to:

\[
g_R(q, p, k) = \frac{1 - \epsilon}{2} A_0(k) \frac{\omega^2}{c^2} - i\{\alpha_0(q)R_1(q, k) + \alpha_1(q)A_1(q, k)\} \quad \text{(B.4)}
\]
\[
g_A(q, p, k) = \alpha_1(k) \frac{1 - \epsilon}{2} A_0(k) \frac{\omega^2}{c^2} + i\left\{\frac{\omega^2}{c^2} - qp\right\} R_1(q, k) - \left[\epsilon(\omega) \frac{\omega^2}{c^2} - qp\right] A_1(q, k) \quad \text{(B.5)}
\]

and
Then the scattering amplitude of $s$- polarized wave will is given by (A.16).
Appendix C

The Article Published in Physical Review B 54, #5, 2980, (1996)
We study by computer simulation an amorphous solid modeled as a percolating cluster of atoms on the fcc lattice. The atoms interact by nearest neighbor Lennard-Jones pair potentials. In contrast to past simulation efforts, the present simulation allows for full three-dimensional motion of the atoms, and exhibits results for the thermal conductivity and density of states of the vibrational modes which differ from previous simulation results. [S0163-1829(96)02029-2]

Though there is a great difference between the temperature dependence and magnitude of the thermal conductivity of crystalline and amorphous insulating solids, the thermal conductivities of amorphous insulating solids are found quantitatively as well as qualitatively to be very similar to one another. In general, three regions of temperature behavior are observed in amorphous insulating solids. These are (1) for $T \leq T_0$, the thermal conductivity exhibits a $T^3$ power law behavior with $T_0 \approx 2$, (2) for $T \approx T_0$, a plateau region is observed in which the thermal conductivity is relatively independent of temperature, and (3) for $T \geq T_0$, the thermal conductivity again exhibits a monotonically decreasing behavior with increasing $T$. As these three features are present in most amorphous insulating solids, exhibiting the same orders of magnitude of the thermal conductivity, a comprehensive theoretical treatment of the thermal conductivity must exhibit these properties for quite general amorphous geometries and atomic interactions.

Recently, computer-simulation work on vibrational excitations and the thermal conductivity of amorphous insulating materials has been done by Sheng and Zhou. They considered a scalar wave treatment (atoms of the system only move in one dimension) of a system of atoms on an infinite percolating cluster (model of amorphous material) defined on a simple cubic lattice.

In this paper we shall present simulation results for the thermal conductivity of a percolating cluster (amorphous material) on which the atoms of the cluster are allowed fully three-dimensional (vector) vibrational displacements. Specifically, atoms in our model are taken to be on an infinite percolating cluster of fcc lattice and to interact by nearest neighbor Lennard-Jones pair potentials. In contrast to past simulation efforts, the present simulation allows for full three-dimensional motion of the atoms, and exhibits results for the thermal conductivity and density of states of the vibrational modes which differ from previous simulation results.

The Hamiltonian of the system we study is

$$H = \sum_{\mathbf{r}, \mathbf{r}'} \sum_{\omega} \left[ \frac{4}{\pi} \delta(\omega) \hat{u}(\mathbf{r}, \omega) \hat{u}(\mathbf{r}', \omega) \right]$$

where $\hat{u}(\mathbf{r}, \omega)$ is the displacement of atom $\mathbf{r}$ at frequency $\omega$, and $\delta(\omega)$ is the delta function. The computation of $\delta(\omega)$ is based on the harmonic approximation using recursive methods. The computation of $D(\omega)$ is based on the full anharmonic Hamiltonian.

Our density of states calculations rely on recursion methods found in the work by Haydock et al. and Nix. For our random network, $\nu(\omega)$ (where $\nu(\omega) d\omega = n(\omega) d\omega$) is the density of states in $\omega^2$, can be written in terms of a summation over the local density of states $n_0(\omega)$ at each atomic site $i$ for the component of atomic motion along the $a$ axis, e.g., $n(\omega) = \sum_i n_0(\omega)$, where $\int_{-\infty}^{\infty} n(\omega) d\omega = 1$. In terms of the dynamical matrix $D$ of the vibrational system

$$n_\omega(\omega') = \frac{1}{\pi} \text{Im} G_{\omega,\omega'}(\omega^2)$$

and $n(\omega)$ is a normalized state of motion of the $i$th atom along the $a$ axis.

Expressing the dynamical matrix $D$ in tridiagonal form

$$D_{mn}^{(n)} = \begin{cases} a_{nn}^{(n)}, & n = m, \\ b_{n+1}^{(n)}, & n = m + 1, \\ b_{n-1}^{(n)}, & n = m - 1, \\ 0, & \text{otherwise}, \end{cases}$$

is the specific heat at temperature $T$ of a vibrational mode of frequency $\omega$, and $D(\omega)$ is the diffusion constant of a phonon of frequency $\omega$. Equation (1) does not make a distinction between the diffusivity of different types of modes of frequency $\omega$, but rather treats all excitations of frequency $\omega$ the same.

The Hamiltonian of the system we study is

$$H = \sum_{\mathbf{r}, \mathbf{r}'} \sum_{\omega} \left[ \frac{4}{\pi} \delta(\omega) \hat{u}(\mathbf{r}, \omega) \hat{u}(\mathbf{r}', \omega) \right]$$

where $\hat{u}(\mathbf{r}, \omega)$ is the displacement of atom $\mathbf{r}$ at frequency $\omega$, and $\delta(\omega)$ is the delta function. The computation of $\delta(\omega)$ is based on the harmonic approximation using recursive methods. The computation of $D(\omega)$ is based on the full anharmonic Hamiltonian.

Our density of states calculations rely on recursion methods found in the work by Haydock et al. and Nix. For our random network, $\nu(\omega)$ (where $\nu(\omega) d\omega = n(\omega) d\omega$) is the density of states in $\omega^2$, can be written in terms of a summation over the local density of states $n_0(\omega)$ at each atomic site $i$ for the component of atomic motion along the $a$ axis, e.g., $n(\omega) = \sum_i n_0(\omega)$, where $\int_{-\infty}^{\infty} n(\omega) d\omega = 1$. In terms of the dynamical matrix $D$ of the vibrational system

$$n_\omega(\omega') = \frac{1}{\pi} \text{Im} G_{\omega,\omega'}(\omega^2)$$

and $n(\omega)$ is a normalized state of motion of the $i$th atom along the $a$ axis.

Expressing the dynamical matrix $D$ in tridiagonal form

$$D_{mn}^{(n)} = \begin{cases} a_{nn}^{(n)}, & n = m, \\ b_{n+1}^{(n)}, & n = m + 1, \\ b_{n-1}^{(n)}, & n = m - 1, \\ 0, & \text{otherwise}, \end{cases}$$

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where $\hat{u}(\mathbf{r}, \omega)$ is the displacement of atom $\mathbf{r}$ at frequency $\omega$, and $\delta(\omega)$ is the delta function. The computation of $\delta(\omega)$ is based on the harmonic approximation using recursive methods. The computation of $D(\omega)$ is based on the full anharmonic Hamiltonian.
The resulting integral for the thermal conductivity depends on the fcc lattice constant $a_0$, $\omega_{max}$, $u$, $A$, and $B$. Values for $u$, $A$, and $B$ are listed in Table I of Ref. 6, and we have taken these over directly in obtaining the result for $K(T)$. To obtain $\omega_{max}$ we have made the approximation $\hbar \omega_{max} = E_D$, where $E_D$ is the Debye temperature listed in Table I of Ref. 6. A value of the lattice constant $a_0$ can be obtained from $a_0 = a/l^3$, where $a$ is the atomic concentration, $l$ is the lattice parameter from Table I of Ref. 6, and $\rho$ is the mass density (taken from Table I of Ref. 6). $a_0$ is the number of atoms in the molecular unit. The $a_0$ is chosen so that the number of vibrational modes per volume is the same in our model as in the experimental material we compare with. In Table I we present parameters we extracted as above for $a$-Se, $a$-SiO$_2$, and PMMA.

In Fig. 3 we present $K(T)$ versus $T$ computed for $p = 0.7$ and $p = 0.8$, respectively. Qualitative agreement is found between the thermal conductivities in Fig. 3 and the experimental data for these materials presented in Fig. 2 of Ref. 6. We do not expect nor do we find quantitative agreement between our Fig. 3 results and the results in Fig. 2 of Ref. 6. This is due to the fact that our model does not reflect the structure of $a$-Se, $a$-SiO$_2$, and PMMA. (Sheng and Zhou in their Fig. 4 choose parameters to force a fit between theory and experiment. We have not done this.)

At $T \approx 1$ K in which the diffusivity is dominated by two level scattering, we find $K(T) \approx T^p$, where at low frequencies $\omega(\omega) \approx \omega^p$. Our results for $p = 0.8$ exhibit Debye behavior for $\omega/\omega_{max} \leq 0.2$. For $p = 0.7$ results, which only exhibit Debye behavior for $\omega/\omega_{max} \leq 0.05$, give $1 < p < 2$. These type of power law behaviors compare favorably with experiment. The scalar wave results of Sheng and Zhou, however, are based on models which exhibit only $p = 2$ Debye like behavior.

The $C_4 \omega^{-4}$ contribution to $D_4(\omega)$ from Rayleigh scattering is important in determining the low temperature limit of the plateau region. This can be seen from Fig. 4. Results are shown for $C_4$, $2C_4$, $4C_4$, and $C_4 \omega^{-4}$ to $C_4 \omega^{-4}$ fit. In the extreme limit that Rayleigh scattering is ignored, a small plateau region is observed even though the thermal conductivity determined in this case is too large. In this limit the plateau region is also observed to begin at too large a value of $T$. For $T > 10$ K, all curves for $K(T)$ eventually increase monotonically with increasing $T$. This behavior follows primarily from the specific heat.

To conclude we find upon comparison with the scalar wave theory the following:

1. Both models exhibit diffusion coefficients which decrease in magnitude with decreasing atomic concentration $p$. The Rayleigh scattering dominates $D_4(\omega)$ at lower frequencies as $p$ is decreased. At lowest frequencies the total diffusivity is determined by two level states scattering.
2. When the frequency is increased a region is observed in which the total diffusivity is dominated by Rayleigh scattering and at the largest frequencies general scattering from the amorphous network is dominant.
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The density of states $n(\omega)$ vs $\omega$ for a system, composed of $N_0$ atoms (atoms on the percolating cluster) for $p = 0.7$, $p = 0.8$, $p = 0.9$, and $p = 1.0$. In this plot, $\omega_{\text{max}}$ is the maximal vibrational frequency of the $p = 1.0$ fcc system. Results for $p = 0.7$ and $p = 0.8$ obtained by directly counting the eigenvalues of the dynamical matrix computed for a reduced array of 864 sites (dashed line histogram results) are also shown.

$G_{ij}(\omega^2)$ can be expanded as a continued fraction,

$$G_{ij}(\omega^2) = \frac{1}{\omega^2 - n_0^i - n_0^j - \frac{1}{\omega^2 - n_0^i - n_0^j - \cdots}}$$

where $\{a^i, b^j\}$ can be calculated using methods similar to those in Ref. 8. In general, we use $20-40$ sets of $\{a^i, b^j\}$ for a given $[i, j]$. The termination used (see Ref. 10 for details) is based on the development of an expression for $n_{ij}(\omega)$ from its continued fraction representation and the derivative of $J_{ij}^0$ with respect to $\omega$.

We have considered a cube of fcc lattice of $21 \times 21 \times 21$ conventional unit cells with periodic boundary conditions. We have determined $n(\omega)$ using 1000 and 6000 different $[i, j]$. Little difference was found between $n(\omega)$ computed using 1000 and 6000. In Fig. 1 we present results for $n(\omega)$ versus $\omega^2$ for $p = 1$, agreeing with Ref. 12. In Fig. 1 results are shown for $p = 0.9$, $p = 0.8$, and $p = 0.7$. Some of these results are compared to results obtained by the counting of eigenvalues of the dynamical matrix for an array of 864 sites.

The phonon diffusion coefficient $D(\omega)$ (proportional to the total mean free path for phonon scattering in the system) is given by $1/D(\omega) = 1/D_{\text{f}}(\omega) + 1/D_{\text{n}}(\omega)$ where $D_{\text{f}}(\omega)$ is for processes involving scattering from a fixed network and $D_{\text{n}}(\omega)$ is for processes involving scattering accompanying a change in network geometry between metastable states. The processes contributing to $D_{\text{n}}(\omega)$ are treated in the context of the two-level state theory, which uses

$$D(\omega) = \frac{1}{l_{\text{f}}(\omega)} + \frac{k_B}{A_{\text{n}}} \left( \frac{h_\omega}{2 \pi N} \right) + \frac{1}{2} \frac{1}{l_{\text{n}}(\omega)}$$

for fitting parameters $A$ and $B$ to give the low temperature behavior of $T\Omega(\omega) = (2k_B)D_{\text{n}}(\omega)$ where $\Omega$ is the average phonon velocity [Eq. (5) was taken from the Ref. 6 and differs from that used by Sheng and Zhou, see Ref. 11].

In computing $D(\omega)$ we study the system dynamics when, to a single atom at the center of the percolating cluster, we apply a time-dependent force of the form

$$F(t) = \begin{cases} F \sin(\omega t) \exp\left(-|yunct|^{2}\right), & t \in [t_0, \infty), \\ 0, & \text{otherwise}, \end{cases}$$

where $|yunct|^{2} \approx 3.8$. The simulation begins at $t = -t_0$. The amplitude distribution of the driving force as a function of frequency in our calculations has a half width at half maximum of $\Delta \omega = 0.07$. It is well known that at low frequencies $D(\omega)$ is dominated by Rayleigh scattering. In Ref. 13, we have used a different form for $\omega$ than that used by Sheng and Zhou, see Refs. 11 and 13.

In Fig. 2 are results for the diffusion coefficient, $D(\omega)$, for $p = 0.55$, $p = 0.7$, and $p = 0.8$. The solid lines in this figure represent $D(\omega)$ computed as described above but the dashed lines represent an interpolation which we discuss below. These results were obtained for percolating clusters created from an fcc region of $37 \times 37 \times 37$ conventional unit cells with periodic boundary conditions.

At the upper frequency limit of $D(\omega)$, we use an interpolation scheme to set $D(\omega)$ to zero at the upper frequency band edge (see Ref. 15). In this case we use a linear interpolation from the upper edge of the simulation computed $D(\omega)$ (solid lines) to zero at $\omega = \omega_{\text{max}}$ for $p = 0.7$ and $\omega = 0.97 \omega_{\text{max}}$ for $p = 0.8$, where $\omega_{\text{max}}$ is the upper band edge of the $p = 1.0$ system.

For the thermal conductivity we use $\kappa(\omega)$, $D(\omega)$, and the specific heat in Eq. (1) to obtain results as a function of $T$. 

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(2) The vector treatment exhibits a density of states which differs considerably from the scalar wave model and accounts for the larger thermal conductivity values observed in our vector treatment. Our results, unlike the Sheng and Zhou results, exhibit a density of states which can depart (except for a very small neighborhood of $\omega = 0$) from a quadratic variation with $\omega$ at very low frequencies.

(3) Both models exhibit the three regions of different temperature dependent behavior observed for $T \approx 100$ K. In both models the plateau region and its lower temperature limit are determined by the Rayleigh scattering from the amorphous network. The exponent $\beta$ in our model offers $1 < \beta < 2$ which is more realistic than $\beta = 2$ observed in the scalar wave treatment.

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Appendix D

The Article Published in Optics Letters, 22, #1, 58, (1997)
A new method known as reverse Monte Carlo (RMC) was recently developed and applied to the determination of the structures of amorphous and polymer materials from x-ray scattering data. This method uses Monte Carlo techniques to generate atomic structures that reproduce the scattering data obtained experimentally from disordered systems and hence act as models for the atomic arrangement in these materials. In this Letter we present a new application of RMC ideas, namely, the determination of the power spectrum of a randomly rough surface from the differential reflection coefficient of electromagnetic radiation scattered from such a surface, i.e., from far-field experimental data.

We consider a randomly rough surface defined by \( z = \zeta(x_3) \), where \( x_3 = (x_1, x_2, 0) \). The surface profile function \( \zeta(x_3) \) is assumed to be a single-valued function of \( x_3 \) that is differentiable as many times as is necessary and that constitutes a stationary, zero-mean, isotropic, Gaussian random process defined by \( \langle \zeta(x_3) \rangle = \langle \zeta(x_3') \rangle = \delta^3W(x_3 - x_3') \). The angle brackets denote an average over the ensemble of realizations of the surface profile function, and \( \delta = \langle \zeta^2(x_3) \rangle^{1/2} \) is the rms height of the surface. The power spectrum of the surface roughness is defined as \( g(k_g) = \int d^3W(x_3) \exp(-i k_g \cdot x_3) \), where \( k_g = (k_1, k_2, 0) \).

The contribution to the mean differential reflection coefficient (mdrc) from the diffuse component of the light scattered from such surfaces depends explicitly on \( g(k_g) \) in those cases when the roughness is weak enough that the mdrc can be calculated perturbatively with the necessary ensemble averages evaluated analytically. It depends implicitly on \( g(k_g) \) when the roughness is strong enough that a computer simulation approach to its evaluation is required.

The RMC method when applied to scattering data from either type of surface works as follows. Let \( [dR_{\text{cm}}(\Omega_i, \Omega_j)/d\Omega_i]_{\exp} \) be the experimental data for the contribution to the mdrc from the diffuse component of the scattered electromagnetic waves when electromagnetic waves of polarization \( \alpha \) and angles of incidence \( \Omega_i \) are scattered into waves of polarization \( \beta \) and scattering angles \( \Omega_j(\sigma, \beta = \rho, \sigma) \), let \( g_0(k_g) \) be an initial guess at the power spectrum, and let \( [dR_{\text{cm}}(\Omega_i, \Omega_j)/d\Omega_i] \) be the contribution to the mdrc computed by theory or computer simulation from \( g_0(k_g) \). Next compute

\[
x_0 = \sum_i \sum_j \int d\Omega_i [\alpha(\Omega_i, \Omega_j)]^{-2} \left[ \frac{dR_{\text{cm}}(\Omega_i, \Omega_j)}{d\Omega_i} \right]_{\exp} - \left[ \frac{dR_{\text{cm}}(\Omega_i, \Omega_j)}{d\Omega_i} \right]_{\text{go}}^2,
\]

where \( [\alpha(\Omega_i, \Omega_j)]^{1/2} \) is the variance of the experimental data about their mean. The sum on \( i \) allows for the use of scattering data from more than one angle of incidence. (The exact power spectrum \( g_0(k_g) \) gives \( x_0 = 0 \) when it is substituted into the RMC method as a guess.) A random change is then made in \( g_0(k_g) \) to create a new guess power spectrum \( g_1(k_g) \), which yields a new differential reflection coefficient \( [dR_{\text{cm}}(\Omega_i, \Omega_j)/d\Omega_i] \), and

\[
x_1 = \sum_i \sum_j \int d\Omega_i [\alpha(\Omega_i, \Omega_j)]^{-2} \left[ \frac{dR_{\text{cm}}(\Omega_i, \Omega_j)}{d\Omega_i} \right]_{\exp} - \left[ \frac{dR_{\text{cm}}(\Omega_i, \Omega_j)}{d\Omega_i} \right]_{\text{go}}^2.
\]

If \( x_1 < x_0 \) then \( g_1(k_g) \) is retained over \( g_0(k_g) \) as a good guess for the power spectrum. If \( x_1 \geq x_0 \) then \( g_1(k_g) \) is retained over \( g_0(k_g) \) with probability \( p = \exp(x_0 - x_1) \). This last step keeps the system from becoming stuck in a local minimum of \( x_1 \) and is based on maximum entropy methods, which choose the most probable solution for \( g(k_g) \) consistent with the experimental data. Otherwise, \( g_0(k_g) \) is retained. The above process is repeated until \( [dR_{\text{cm}}(\Omega_i, \Omega_j)/d\Omega_i]_{\exp} \)

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As a result, the power spectrum scattering theory.

data (see, e.g., Ref. 12) are based on a single-scattering spectrum of a randomly rough surface from measured results for the mdc of light scattered diffusely from randomly rough surfaces. Existing methods for obtaining the power spectrum from diffuse scattering data (see, e.g., Ref. 12) are based on a single-scattering approximation to the mdc, which could not be used in reconstructing the West–O’Donnell power spectrum because it produces surfaces from which single-scattering processes are largely suppressed.11 The RMC method in the present study is based on a theory that involves the multiple scattering of surface waves. As a result, the power spectrum \( g(k) \) can be obtained for a larger range of \( k \) than is possible with a single-scattering theory.

In addition, the RMC method contains two important improvements over routines that compute \( g(k) \) by a straightforward minimization of \( \chi \) (Ref. 13): (1) the Monte Carlo component of the RMC offers an efficient way to minimize \( \chi \) approximately and (2) the maximum entropy component of the RMC sorts out from all the local minima of \( \chi \) the most probable solution for \( g(k) \). In this regard, the more scattering data (more experimental points and more angles of incidence) used, the more probable is the agreement of the \( g(k) \) computed by the RMC with the actual \( g(k) \).

It is important along with a study of the convergence of the RMC routine itself to study the change in the computed \( g(k) \) as data from additional angles of incidence are added. Data from two angles of incidence were needed to achieve the accuracy displayed in the figures. The use of data taken at more angles of incidence should improve the computed \( g(k) \).

The method that we have presented is readily generalized to treat surfaces that are defined by surface profile functions that are not Gaussian random processes. One generalization of the RMC method described here that we are currently pursuing is the extraction of deterministic surface profiles from scattering data. Here the differential reflection coefficient is expressed in terms of the surface profile function \( \xi(x) \), and the random guesses in the RMC method are made of \( \xi(x) \) rather than of the power spectrum as in the random surface RMC.

When an analytic result for \( \langle \sigma R(\theta, \psi) / d\psi \rangle \) is not available, the RMC method can still be used to determine the power spectrum \( g(k) \), at the expense of additional computational effort. For each choice of \( g(k) \) an ensemble of several hundred profiles would have to be generated by a standard method,6,7 the results for \( \langle \sigma R(\theta, \psi) / d\psi \rangle \) for each member of the ensemble would have to be averaged, and the result would have to be used in the RMC algorithm.

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Permanent address, A. F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia.

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Appendix E

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Speckle correlations in the light scattered from a weakly rough one-dimensional random metal surface

V. Malyshkin* and A. R. McGurn

Department of Physics, Western Michigan University, Kalamazoo, Michigan 49008

T. A. Leskova

Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow District 142092, Russia

A. A. Maradudin

Department of Physics and Astronomy, and Institute of Surface and Interface Science, University of California, Irvine, California 92697

M. Nieto-Vesperinas

Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Científicas, Cantoblanco, Madrid 28049, Spain

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Perturbation theory is used to compute the angular-intensity correlation function \( C(q, kq', k') = \langle l(q|k) \rangle / \langle l(k|q') \rangle / \langle l(q|k') \rangle \) for \( p \)-polarized light scattered from a weakly rough, one-dimensional random metal surface. \( I(q|k) \) is the squared modulus of the scattering matrix for the system, and \( q, k, k' \) are the projections of the mean scattering surface of the wave vectors of the scattered and the incident light, respectively. Contributions to \( C \) include (a) a short-range memory effect and time-reversed memory effect terms, \( C^1(q, kq', k') \); (b) an additional short-range term of comparable magnitude \( C^{11}(q, kq', k') \); (c) a long-range term \( C^\infty(q, kq', k') \); (d) an infinite-range term \( C^\infty(q, kq', k') \); and (e) a new term \( C^{11}(q, kq', k') \) that along with \( C^\infty(q, kq', k') \) displays peaks associated with the excitation of surface polarizations. These new features arise when the factorization approximation is not made in calculating the correlation function \( C \).

Interest in the angular-intensity correlation function of light scattered from randomly rough surfaces has been growing recently. Multiple-scattering theories of such correlation functions for electromagnetic waves scattered from disordered volume systems led to the prediction of a number of novel features, some of which were observed experimentally. It is of interest to explore whether their analog exist in rough-surface scattering.

For a one-dimensional random surface the angular-intensity correlation function is defined as

\[
C(q, kq', k') = \frac{\langle l(q|k) \rangle \langle l(q'|k') \rangle}{\langle l(k|q') \rangle},
\]

(1)

where \( l(q|k) = (\omega/c)S(q|k)L \), \( S(q|k) \) is the scattering matrix for the scattering of light the projection of whose wave vector on the mean scattering surface is \( k \) into light the projection of whose wave vector on the mean scattering surface is \( q \) and \( L \) is the length of the mean surface along the \( x \)-axis. The angle brackets denote an average over the ensemble of realizations of the random surface. The angle of incidence \( \theta_0 \) and the scattering angle \( \theta \) are given by \( k = (\omega/c) \sin \theta_0 \) and \( q = (\omega/c) \sin \theta \), respectively, for light of frequency \( \omega \).

The correlation function \( C \) was investigated in several analytic and computer simulation studies of scattering from one- and two-dimensional random surfaces. These studies predicted the memory effect and the time-reversed memory effect contributions to \( C \), denoted by \( C^1(q, kq', k') \), which are of the form

\[
C^1(q, kq', k') = 2\pi \delta(q - k - q' + k')C^0(q, kq', k'),
\]

These effects have been observed experimentally. We present results for other contributions to \( C \) that to our knowledge have not been considered theoretically or experimentally: a new short-range correlation function \( C^{11}(q, kq', k') = 2\pi \delta(q - k - q' + k')C^{11}(q, kq', k') \) and two long-range correlation functions, \( C^{11}(q, kq', k') \) and \( C^{11}(q, kq', k') \), which place no restrictions on \( q, k, q' \), and \( k' \) but exhibit novel resonances related to surface polarizations that were not previously noted. These new features are a consequence of our not having invoked the factorization approximation. We also make suggestions regarding types of random surface that are favorable for the observation of these new phenomena.

Consider a weakly rough one-dimensional surface whose profile is given by \( f(x) \), where \( f(x) \) is a single-valued function of \( x \). The surface is stationary with the mean height of the surface being zero. The region \( x > (x_0) \) is vacuum and the surface is imperfect for \( x < (x_0) \). The region \( x > (x_0) \) is a metal of dielectric constant \( \varepsilon \) of which the surface is a perfect conductor with thickness \( x < (x_0) \).

The light in the system is \( p \)-polarized, and for \( x > (x_0) \), the magnetic field is

\[
H_x(x) = \exp\{ikx - i\alpha_0(k)x_1\} + \int_{x_1} \frac{dq}{2\pi} \frac{S(q|k)}{\alpha_0(q)} \times \exp\{iqx + i\alpha_0(q)x_1\},
\]

(2)
where \( \alpha_0(q) = (\omega^2/c^2) - q^2/2 \), Re \( \alpha_0(q) > 0 \), Im \( \alpha_0(q) > 0 \). Following Ref. 9 we have

\[
S(q|k) = -2\pi \delta(q - k) - 2i\alpha_0^2(q)G(q|k)\alpha_0^2(k),
\]

(3)

where the surface polariton Green's function \( G(q|k) \) is the solution of the Dyson equation

\[
G(q|k) = 2\pi \delta(q - k)G_0(k) + G_0(q) \int_{-\infty}^{\infty} \frac{dp}{2\pi} \times V(p)G(p|k).
\]

(4)

\( G_0(k) = i\epsilon(\omega)/[i\epsilon(\omega)\alpha(k) + \alpha(k)] \) is the surface polariton Green's function for a planar vacuum–metal interface, the scattering potential \( V(q|k) \) for small roughness is \( V(q|k) = [(\epsilon(\omega) - 1)\epsilon^2(\omega)]/(\epsilon - k)(\epsilon - q - k) - \alpha(q|k) \), and \( G(p|k) = \int dx \exp(-ipx) \times \xi(x) \), while \( \alpha(p) = (\epsilon(\omega)^2/c^2 - p^2)^{1/2} \), with Re \( \alpha(p) \), Im \( \alpha(p) > 0 \). In terms of \( G(q|k) \)

\[
C(q,kq',k') = (\omega/c)^6 \alpha_0(q)\alpha_0(k)\alpha_0(q')\alpha_0(k') \times D(q,kq',k'),
\]

(5)

where \( D(q,kq',k') = (G(q|k) - G(q|k))G(q'|k') - G(q'|k') \),

To obtain \( G(q|k) \) as an expansion in powers of \( \xi(x) \). In calculating \( D \) we omit specular contributions, for which \( q = k \) and (or) \( q' = k' \).

We present results for \( C \) calculated for a random surface characterized by a power spectrum (defined as \( g(Q) = \int dz W(zr) \exp(-Qz^2/4) \)) that has the Gaussian form \( g(Q) = \sqrt{\pi} a \exp(-Q^2a^2/4) \), where \( a \) is the transverse correlation length of the roughness, as well as for a surface characterized by a power spectrum given by \( g(Q) = (\pi/\Delta k) \text{rect}(Q - K_{\text{mc}}Q)/\Delta k \) + \text{rect}(Q + K_{\text{mc}}Q)/\Delta k), where \( \Delta k = 2(\omega/c) \sin \theta_{\max} \), \( K_{\text{mc}}Q = [\omega(\omega)/\text{Re}(\epsilon(\omega))[1+1]]^{1/2} \) is the wave number of surface polaritons of frequency \( \omega \) at a planar vacuum–metal interface, and \text{rect} denotes the rectangle function. The latter type of surface was used recently and its use increased the strength of the enhanced backscattering from the surface polariton mechanism by an order of magnitude more than that for a surface with the same rms height and rms slope characterized by a Gaussian power spectrum.

In Fig. 1, we plot the contributions to the angular-intensity correlation function when light of wavelength \( \lambda = 612 \text{ nm} \) is incident upon a randomly rough gold surface \( \epsilon(\omega) = -9.9 + i1.29 \) characterized by a West–O’Donnell power spectrum for which \( \delta = 10.9 \text{ nm} \) and \( \theta_{\max} = 13.5^\circ \) and upon a gold surface characterized by a Gaussian power spectrum for which \( \delta = 10.9 \text{ nm} \) and \( \alpha = 129.1 \text{ nm} \). The two random surfaces thus possess the same rms height and slope. In Figs. 1(a) and 1(b) we plot \( LC_{\text{mc}}(q,klq',q' - q + k) \) and \( LC_{\text{mc}}(q,klq',q' + q - k) \), respectively, as functions of \( \theta_0 \) for \( \theta_0 = 1^\circ \) and \( \theta_0 = -5^\circ \). The dominant contributions to these functions come from the terms of fourth and sixth orders in \( \xi(x) \) in \( D \). The function \( C^{10} \) has peaks at \( q' = q \) (memory effect) and at \( q' = -k \) (time-reversed memory effect) and demonstrates that an angular shift of the incoming beam causes the same angular shift of the entire speckle pattern. The function \( C^{12} \) arises because we have not used the factorization approximation in calculating \( D \) and reflects the symmetry of the speckle pattern with respect to the specular direction.

In Fig. 1(c) we present the contribution of what to \( C \), which we have denoted by \( C^{12} \); this contribution arises first in the contribution to \( C \) of sixth order in

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The contribution of \( C \) is plotted as a function of \( q' \) for \( \theta_0 = 1^\circ, \theta_0' = 9^\circ, \) and \( \theta_0 = -5^\circ. \) The function \( C_{1S} \) displays peaks that arise from a factor of \( |G_0(z)|^2, \) where \( z = q'(z - k'), k'(z - k), q = (q' - k'), \) or \( k = (z - k'), \) which has peaks when \( z = z_{kp}. \) In Table 1 we present the wave-number conditions for the peaks in Fig. 1(c). The correlation function \( C_{1S} \) decays slowly as a function of \( s \) and can be regarded as exhibiting long-range correlations between speckle patterns. The features of \( C_{1S} \) are dominated by scattering processes involving surface polaritons. \( C_{1S} \) vanishes in the factorization approximation.

In Fig. 1(d) we plot \( C_{0}(q, k, k', q') \) as a function of \( q' \) for \( \theta_0 = 1^\circ, \theta_0' = 9^\circ, \) and \( \theta_0 = -5^\circ. \) The dominant contribution to \( C_{0} \) comes from terms in \( D \) of eighth order in \( \xi(z). \) This contribution displays peaks arising from factors such as \( G_0(q)G_0(s - \rho), \) where \( \rho \) is an integration variable and \( z \) is a linear combination of \( q' \) and some combination of \( k, k', \) and \( q. \) This factor possesses a Lorentzian peak in \( z \), independent of \( \rho, \) and arises from scattering processes involving surface polaritons. The strongest peaks occur at values of \( q' \) given by \( q' = z_{q}, q' = z_{k}, q' = z_{k'}. \) Analogous peaks were found in the correlation function \( C_{1S} \) for scattering from bulk disordered media, and these peaks had a similar origin. The wave numbers for the peaks in Fig. 1(d) are presented in Table 1.

From the results in Fig. 1 it can be seen that the height of the peaks in \( C_{1S}, C_{1S}, \) and \( C_{0} \) for the surface characterized by the West–O’Donnell power spectrum are enhanced by roughly two orders of magnitude over those for the surface characterized by the Gaussian power spectrum. However, the narrow bands of wave numbers for which the West–O’Donnell power spectrum is nonzero limit the range of \( \theta'_0 \) within which peaks in \( C_{1S}, C_{1S}, \) and \( C_{0} \) can occur. The Gaussian power spectrum is nonzero for all wave numbers and, in general, gives rise to more peaks over a wider range of \( \theta'_0 \) than does the West–O’Donnell spectrum.

As does volume scattering, rough-surface scattering displays infinite-range correlations, the so-called \( C_{1S} \) correlations. The corresponding contribution to \( C \) is a structureless function of \( q' \) for given values of \( k, k', \) and \( q, \) and we do not present a plot of it.

A careful analysis of the \( C_{1S} \) and \( C_{1S} \) correlation functions shows that the ratio of the heights of the peaks of the latter function to the heights of the peaks of the former function is of the order of \( I/I_s, \) where \( I_s \) is the amplitude mean free path of surface polaritons due to ohmic losses in the metal substrate. However, if the incident fields, which we represent with plane waves, are replaced by Gaussian beams of half-width \( w, \) the ratio of these peak heights becomes of the order of \( I/I_s, \) independent of the length of the rough surface. For the wavelength of the incident light used in the present calculations, and the corresponding dielectric constant, we find that \( I_s = 60.23. \) This means that for a focused beam for which \( w \) is of the order of 5000 \( \mu \)m, \( C_{1S} \) can be considerably smaller than the ratio of the heights of the peaks in \( C_{1S} \) to those in \( C_{1S} \) will be approximately 1/8 and hence should be experimentally observable.

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*On leave from A. F. Ioffe, Physical–Technical Institute, St. Petersburg, Russia, 194021.

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