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TRANSPORT IN SMALL AND/OR RANDOM SYSTEMS

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INTRODUCTION

(a) Technological Importance

The introduction of molecular beam epitaxy¹ (MBE) and metallo-organic chemical vapor deposition² (MOCVD) has permitted the engineering of heterostructures from multilayer cases to single quantum wells. The additional procedure of modulation doping introduced by Stormer, Dingle, Gosard and Wiegmann³ has permitted mobilities of the order of $10^6 \text{ cm}^2 / \text{V sec}$ to be attained. "Band structure engineering" has also enhanced the possibilities for construction of semi-conductor lasers.

A large number of devices based on these techniques has caused the physics of film heterostructures to be a field of intense study.⁴

Among the topics of interest to us are hot electron effects, electron-phonon interactions and resonant tunneling. As the dimension of devices shrink, ordinary voltages lead to strong fields and hot electrons. They also lead to devices whose dimension is not much larger than the mean free path. Thus ballistic, or quasi-ballistic transport becomes important.

(b) Transport in Small Systems

We have recently explored the transport of phonons in GaAs at sufficiently low temperatures that the slab thickness is just several mean free paths.⁵ Our Monte Carlo results, in the regime in which down-conversion can be neglected, have led to sufficient insight to lead to a useful, approximate analytic model. These results should be of use in other problems as the transition is made from diffusive to ballistic transport. A copy of a preliminary report is enclosed.

(c) Quasi - 2D Systems

Electron-phonon interactions in a single quantum well, or in a heterostructure can, to a first approximation be regarded as an interaction between a two-dimensional (2D) electron and three-dimensional (3D) phonons. This remark also applies to electrons (or holes) in inversion layers or MOS structures. Peter Price⁶ recognized that physical answers in such a situation depend on the effective number of phonon modes that coupled in, and that this number appears to depend on the arbitrary choice of quantization volume.

Cai, Marchetti and I⁷ have shown that this problem can be solved by coupling the electrons to wave-packets of phonons that are localized in the vicinity of the quantum well. But what shape

should be chosen for the phonon packets? A method Bogolyubov developed years ago for dealing with transport in fluids was employed. This method introduces a small number of "macroscopic" variables and adiabatically eliminates the remaining variables. The result is a reduced transport equation for the slow variables.

An important physical decision must be made as to what the appropriate "macroscopic" variables are. The choice we made for the slow variables was the reduced one-body density matrices of both the electron and phonon gas. The beauty of this choice is that it permits one to retain off-diagonal elements in q_z and q'_z , the components of wave vector perpendicular to the well walls. Thus no choice has been made for the shape of the wave packets.

Because the kernel of the integral equation for the phonon density matrix is found to be a product (more precisely a sum of four products) the natural procedure for solution of such an integral equation leads to the phonon packet representation. Moreover, there is one choice of packet for each quantum well state. Thus at low temperatures in which only a small number of well states are occupied, the number of equations is equal to the number of well states occupied. This good fortune means that the coupled integro-differential equations are reduced to a trivial number of coupled ordinary differential equations. In this way, a rigorous approach to the paradox raised by Price also leads to a practical method of solution.

Having broken the Gordian knot of the proper method of coupling 2D electrons to 3D phonons, the solution of many problems of interest are possible. We have already reported, in the above paper, on non-equilibrium electron-phonon scattering in heterojunctions. Because the electrons coupled into individual phonon packets, the equilibrium of these packets is appreciably disturbed, a back-reaction sets up, and the steady state energy loss rate of a hot electron can be greatly reduced. A second calculation by Cai, Marchetti and Lax³ solves the associated problem of time-dependent electron relaxation. Additional problems involve a strong electric field, multi-subband occupation and transport in the presence of a magnetic field.

The work on quasi 2-D systems will be the subject of an invited paper at the next international conference on Hot Electrons in Semiconductors.

(d) Noise In Small Systems

Because noise may be an important factor in the limits of achievement of small systems including heterostructures and semiconductor lasers, we purpose to consider the development of tools to calculate this noise. Although we already have an arsenal of tools on classical noise⁹⁻¹⁴ and

quantum noise,¹⁵⁻²⁷ we expect that new techniques must be developed because of the quasi-2D nature of some systems, and quantum nature of the motion perpendicular to the heterostructure walls.

We have already seen that transport in electron-phonon systems in non-equilibrium requires the use of density matrices and appropriately determined phonon wave-packets. The same will clearly be true for noise in such systems.

(e) Laser Propagation in the Atmosphere

The random problems associated with propagation through a random medium containing particulate scatterers including aerosols are well-known, but the emphasis has been on solutions for an incident plane wave. The problem of dealing with an incident Gaussian beam, initially narrow in both angle and transverse dimension has only recently been attempted. See Zardecki and Gerstl,²⁸ Chitanvis.²⁹ The need for a comprehensive treatment is clear.

(f) High Intensity Laser-Aerosol Interactions

When a laser beam has high intensity, its interaction with an aerosol becomes nonlinear. Shocks and rarefaction waves can form at high powers. Evaporation will be important at lower powers and longer times. Such problems require a numerical treatment on a large computer because of their hyperbolic character and dependence of two space and one time variable. However, solution of special cases e.g. of planar or spherical symmetry to provide tests of the available 2D hydrocodes are desirable.

We propose to make use of CAVEAT,³⁰ recently written 2D hydrocode involving a half-dozen authors over several years at Los Alamos. A strong point of this code is that it permits the handling of shocks by treating each cell side as if it were a potential discontinuity boundary. It then applies Godonov's procedure treating each discontinuity as if it involved an infinite plane and uses the Riemann scaled solution of the latter problem.

I have questions concerning the accuracy with which the code accurately reflects Godonov's original ideas (as opposed to his original algorithm). Also Chitanvis has suggested, and I agree that the scaling assumption in the Riemann solver is no longer valid when thermal energy is released into the system. The problem, therefore, is to see if corrections incorporating the new physics can be incorporated into the code without changes that would disturb its otherwise excellent features.

(g) Reflection From Random Surfaces

An improved theory of scattering from rough random surfaces will be attempted that includes correlation effects on the surface and multiple scattering.

Somewhat more detailed description of the previous success, and proposed new work on the topics mentioned above, are included in the sections written below by my students and research associates. A detailed discussion is given below.

TRANSPORT PROPERTIES OF CARRIERS IN SEMICONDUCTOR QUANTUM WELL (Cai and Zheng)

1. Nonequilibrium phonon effect on hot carrier transport

Recent experiments have shown that the presence of nonequilibrium optical phonons induces important effects on hot carrier properties in semiconductor quantum wells. We have proposed a description of hot phonon dynamics in quantum-well structures that properly treats the coupling of 2D - carriers and 3D lattice excitations⁷. Our approach rests on the derivation of a phonon kinetic equation that applies in the presence of the strong spatial inhomogeneity due to carrier confinement and on the introduction of a "phonon wave packet" representation. We used this approach to evaluate the effect of nonequilibrium optical phonons on relaxation of hot electrons in heterojunctions both in a steady state⁷ and in a time dependent situation⁸. A reduction of the electron cooling rate of a factor 6-8 was obtained in the steady state case. The suppression of hot electron cooling is even stronger in the time dependent case. Both results are in agreement with recent experiments.

Since the presence of nonequilibrium optical phonons can greatly affect the distribution function of electrons in their relaxation process, various electron properties are changed due to this effect. Previous theoretical results, most of which are calculated based on the assumption that phonons are in equilibrium with heat bath, should be reexamined.

Recently we are studying the effect of nonequilibrium optical phonons on hot electron transport in heterojunctions in the presence of a uniform external strong electric field E . Scattering with remote impurities and acoustic phonons via both deformation potential and piezoelectric interaction are included. The decay of the nonequilibrium LO phonons is described by a single relaxation

time. Our initial results show that there are important effects on the electron transport due to presence of hot phonons. We find that reabsorption of nonequilibrium optical phonons increases the weak field-electron mobility. At high field the presence of nonequilibrium optical phonons enhances electron temperature much faster with the field than that in the case of equilibrium phonons and the mobility normalized to its weak field value decreases faster with the field than obtained when the LO phonons are in equilibrium. The occupation number of nonequilibrium LO phonons is strongly anisotropic in the direction of electric field. We also study the time dependent evolution process after applying an electric field. We find the time needed for approach to the steady state in the presence of hot phonons becomes much longer than that in the equilibrium phonon case.³¹

A drifted temperature model and a single subband approximation, however, are used in our recent calculation. A more detail computation, which includes multi-subbands and multi-valleys is needed, especially, for the case that a high electric field is applied. A calculation of cooling rate of hot electrons in the case where the multi-subbands are occupied has been worked out,³² which shows that our description of "phonon wavepacket" can be used in multi-subbands case without difficulty.

Recently, we are also studying the nonequilibrium phonon effect on transport of holes in quantum wells.

2. Transport of an electron-hole gas in a quantum well

Recently there has been much interest in the 2D semiconductor system where the electrons and holes coexist. The experiments have shown that when a strong electric field is applied to this system, the electrons and the holes have different drift velocities and different temperatures.³³ Under some special conditions it has been discovered that the electrons can move along positive direction of the external electric field.³⁴ Namely, an absolute negative mobility of electrons is shown. In addition to the scattering of electrons and holes with phonons and impurities, the electron-hole scattering plays a important role in the transport of this system, which produces the "electron-hole drag" effect.

We address to the transport phenomena in this system. the dynamic screening effect in this system has a special form since electron-hole interaction is as important as electron-electron (hole-hole) interaction. Also this screening effect make the coupling of electron-phonon (impurity) interaction with hole-phonon (impurity) interaction. The subband wavefunctions of electrons and holes in this system are different from the case that only electrons (or holes) exist, because the common self-consistent potential is a superposition contributed from both electrons and holes. To our knowledge, these have not been carefully considered before. We have also derived a set of coupling equations to obtain temperatures and mobilities for both electrons and holes. The conditions of the absolute

negative mobility of electrons we obtained is different from what shown in previous paper by other authors.³⁴ The numerical computation is in progress.

WORK NEAR COMPLETION

(1). Scattering from correlated points of a random rough surface

EM wave scattering from a random rough surface arises in many areas of science and engineering, such as atomic scattering from a solid surface, and remote sensing for Earth terrain. When the correlation length and variance of roughness are much larger than the wavelength, the Kirchhoff approximation is applied. The variables of the roughness: heights and slopes of the specular points, have previously been dealt with as independent. Therefore, the contribution from such correlation was totally omitted. In the high frequency limit, the scattered intensity finally is only a summation from independent stationary points.

However, our study elucidates that for any pair of specular points in one Fresnel zone, as long as their distance is not larger than the correlation length (note that the latter might be much larger than the wavelength), the roughness heights and slopes are correlated. Note that most contribution to the scattered intensity happen to come from this small region. The contributions from these correlations are appreciable, and should be taken into account for computation of the scattered intensity. A general approach and analytic formulation to take account of the correlation have been developed. The difference caused by the correlation is discussed, and numerical results are also provided in the manuscript.

(2). Multiple scattering from a randomly rough surface

Solution for scattering from a randomly rough surface has been achieved by the well-known methods of Kirchhoff approximation, small perturbation theory^{47,48}, and recently by the full wave⁴⁹ approach, and others. However, these approaches generally are restricted to the single scattering approximation. Multiple interactions of a scattered wave with the surface were disregarded. The multiple scattering theory for a randomly rough surface (mostly, for a perfect conducting surface) has been discussed by using a diagrammatic method,⁵⁰ Stochastic Fourier transformation, smoothing^{51,52} method, etc. However, these discussions are largely formal, and the emphasis is on the analytic structure of the integral equation of scattered field. These methods do not seem to be tractable enough yet to quantitatively assess the effect of multiple scattering.

We wish to develop an explicit formula to take multiple scattering into account. The polarized scattered power from a randomly rough surface is contributed to not only by single scattered waves, but also by those high order scattered waves which undergo re-incident and re-bounced

scatterings in various directions. The multiple scattered field is represented as a Born series. By using the stationary phase method, the scattered field with the single scattering assumption has been previously obtained. For the double scattering, the scattered power is contributed by those statistically distributed pairs of the stationary points, which are illuminated, not obscured, and there is no obstacle between them. Shadowing functions are obtained by making use of the method of random variable overshoots to the determinant ray. The polarized scattered fields for double scattering can be expressed by the sequential-scatterings (second-order Born approximation) and shadowing factors. Then, an explicit formula for the bistatic double scattering intensity can be statistically obtained, and by iteration the higher order scattering can be estimated. Thus, the contribution to the polarized scattered power from high order scattering from a randomly rough surface with given statistics can be evaluated. Functional dependence of the scattering and numerical calculations are obtained, and discussed in the manuscript.

LIGHT TRANSMISSION IN A PARTICULATE MEDIUM (B.Yudanin)

Light propagation through an optically thick particulate medium is basically a multiple - scattering problem in which rays or photons traverse a medium of scatterers and undergo many scattering events before escaping. A natural framework to deal with this type of problem is provided by the theory of radiative transfer. The linear Boltzman equation - in the context of radiative energy also termed the equation of transfer - governs the radiation field in a medium that absorbs, emits, and scatters radiation.

The complexity of the equation of transfer forces one to implement numerical methods of solution. Unfortunately, such calculations become a rather formidable task even on the most powerful supercomputers available today.

Due to the numerical complexities, an important aspect of transport theory involves development of simpler approximate descriptions. The well-known small-angle approximation procedure provides an example of the algorithm applicable to scattering from particles with highly anisotropic phase function. When the particle density is sufficiently tenuous, a single-scattering approximation is adequate. When the scattering is nearly isotropic, a diffusion approximation becomes adequate even in the presence of absorption. With moderate anisotropy, the quantitative measure of which is the mean cosine of the scattering angle, the diffusion approximation gives relatively simple and good solutions when the particle volume density is high. Of course, the diffusion equation will contain the necessary absorptive term.

One way to simplify the transport equation is to reduce it to a form of three simultaneous

partial differential equations for the reduced field amplitude, the forward- and backscattered irradiances. The scattering and diffusion coefficients in these equations will be defined in terms of Mie functions. The determination of those coefficients will be one of the main aspects of our investigation. The theory which we are planning to develop will be based on multiple-scattering theory.

As a starting point in our investigation we consider the correlation function of the electric field of the radiation of frequency ω and velocity c .

$$\Gamma(\mathbf{R}, \mathbf{r}, \Omega, \omega) = \overline{E(\mathbf{R} + \frac{\mathbf{r}}{2}; \Omega + \frac{\omega}{2}) E^*(\mathbf{R} - \frac{\mathbf{r}}{2}; \Omega - \frac{\omega}{2})} \quad (1)$$

The Fourier transform of Γ with respect to $\mathbf{r}$ and ω is proportional to the intensity of radiation at $\mathbf{R}$ with wave vector $\mathbf{q}$. This quantity can be expressed in terms of the average of the product of two Green's functions.

To get a generalized transport equation for the intensity of the radiation in the presence of randomly distributed scatterers we will first obtain an integral equation for the correlation function Γ in the approximation which is consistent with a CPA for the average field E .

First we introduce the coherent dielectric constant ϵ_c and the coherent Green's function G_c , such that there will be no scattering on the average from such a media (e.g., the average T -matrix is zero). This will lead to the condition that the average Green's function of the field is equal to the coherent one. The coherent potential and the corresponding coherent Green's function can be found self consistently as was done in any standard C.P.A calculation for, say, liquid-type disorder.

As stated above, to find intensity we need to know the average of the product of two Green's functions at different space-time points. An equation, consistent with the C.P.A for the average of the product of two Green's functions will contain as a kernel an average of the product of the t -matrices for the scatterer, imbedded into otherwise coherent medium

After some manipulations arrive into a familiar form of a differential transport equation:

$$\begin{aligned} i \left[\omega \frac{\partial}{\partial t} + \mathbf{q} \cdot \nabla \right] \Gamma^{nc}(\mathbf{R}, \mathbf{q}, t) + \frac{1}{2} \int d\mathbf{R}' \Delta V_c(\mathbf{R} - \mathbf{R}', \mathbf{q}) \Gamma^{nc}(\mathbf{R}', \mathbf{q}, t) \\ = \frac{1}{2} \int \int \int \int dt' d\mathbf{R}' d\mathbf{q}' d\mathbf{Q} \Delta G_c(2\mathbf{q}', \mathbf{q}, t - t') e^{-i(\mathbf{q} \cdot \mathbf{R} + \mathbf{Q} \cdot \mathbf{R}')} \\ \times t(\mathbf{q} + \mathbf{q}', -\frac{\mathbf{Q}}{2} - \mathbf{q}') t^*(\mathbf{q} - \mathbf{q}', \frac{\mathbf{Q}}{2} - \mathbf{q}') \Gamma(\mathbf{R}', \mathbf{q}', t') \end{aligned} \quad (2)$$

To get a set of equations for the intensities and amplitudes of the form of the diffusion and the small

angle transport, we will decompose the t -matrix for the scatterer into a small angle part and the uniform (large angle) part, which will be separately responsible for the arising paraxial and diffusion equations for the transport. It seems to be reasonable to incorporate the wide angle scattering into a new "coherent medium", and to keep the small angle part of the scattering in the kernel of the equation (2).

In our following work we plan to simplify this full transport equation to the form of coupled equations for the small angle and for the diffusion scattering. We also plan to get a numerical solution of that system of equations.

LASER GENERATION OF SHOCK WAVES IN DROPLETS (C. L. Wang)

The generation of shock waves in droplets by laser beam illumination has been studied in recent years. The droplets are first heated up by irradiation of laser beams, then expand and explode, producing shock waves and rarefaction waves. The problem is involved in two aspects, electrodynamic and hydrodynamic. The first aspect is to consider the interaction between electromagnetic waves and small droplets which causes the energy transfer from laser beams to water droplets. This procedure is governed by Maxwell equations. The second aspect is to investigate hydrodynamical response which is determined by a set of conservation equations (mass, momentum and energy). The two set of equations are strongly coupled through source terms in the primitive equations and through the constitutive relations.

The feedback amongst the various electromagnetic and hydrodynamical equations can give rise to very unusual behavior. In fact, in computer simulations one might be hard pressed to distinguish the true physical behavior from numerical rubbish. However, the two very different aspects of the problem suggest that much can be learned by attacking them separately at the start. For example, the hydrodynamic equations can be solved assuming the absorption of laser radiation is known.

We propose to emphasize first the hydrodynamical aspects of this problem. To a first approximation, the effect of EMR on a small droplet is to generate heat within the droplet due to absorption. The rate at which the heat is generated determines the response of the droplet. The heating can vary over a wide range as determined by the complex index of refraction, the intensity of the radiation source, and the optical size of the droplet. The droplet shows an equally wide range of response, from slow evaporation to explosion.

A large body of literature has developed considering many aspects of this problem. For example, the articles by Caris and Brock⁵³, Lax and Yudanin⁵⁴, Prishivalko⁵⁵, and Chitanvis⁵⁶ illustrate

the wide range of effects that are being considered. Most of the current work addressing a realistic simulation of the hydrodynamics has dealt with the slow vaporization regime (see, for instance, Armstrong^{57,58} and Sageev⁵⁹).

We will work on the explosive vaporization regime of this problem. In this regime convective effects dominate diffusive effects. Convective effects are driven by an imbalance in pressure field. Convection becomes important when the vapor pressure of the evaporating droplet becomes comparable to the pressure of the surrounding gas. Under these conditions, the rate of evaporation is greater than the rate at which diffusion can "conduct" mass away from the droplet. As the temperature and, therefore, the vapor pressure and the evaporation rate of the droplet rise, convection becomes an effective mechanism for the mass transport away from the droplet. At higher temperatures it becomes the dominant mechanism.

We propose to choose a simple but very dynamic test problem as a first step towards developing a general solution for the convection dominated regime. By choosing a relatively simple hydrodynamical system, we can concentrate on simulating the physical properties of the droplet realistically. This in turn will help us determine what other physics (such as nucleation and particle growth) might arise due to strong convective effects. The problem that we are planning to solve can be posed as follows: a pure water droplet, small compared with the wavelength of the incident light, is subject to a very short, very intense pulse of laser radiation. The optical size of the droplet is in the Rayleigh limit, thus it absorbs energy uniformly. In one special case, the very short duration of the pulse can ensure that the heating process ends before any fluid motion occurs. This implies that the droplet heats at constant volume.

Heating the droplet at constant volume causes its pressure to increase enormously (as high as 3000 atmospheres). The high pressure causes the droplet to expand violently against the atmosphere. The strong dynamics generate shock waves and associated shock heating in some regions, and adiabatic expansion, cooling, and the possibility of nucleation in other regions. We plan to consider all these possibilities in our work.

A Lagrangian-Eulerian rezoning code, CAVEAT³⁰, from Los Alamos is in the development stage, which can numerically solve the equations of transient, multimaterial, compressible fluid dynamics. This code employs the Godunov technique, which allows close coupling between cell-centered pressure and velocity fields and serves as the basis for handling jump discontinuity between regions of fluid. The ingenious Godunov method has the virtue of treating any real discontinuity the fluid may contain more realistically than other known methods including the viscosity methods do, because the methods eventually treat each mesh point as if it has a discontinuity. But the Godunov

method essentially makes use of the Riemann solver, which came from an analytically solvable one-dimensional tube problem. The Riemann solver is based on a scaling assumption not valid in the presence of source terms. The applicability of the unmodified Godunov method must be examined. In the mean time, we try to do a parallel test. We plan to modify our existing code, which uses the POST package, to calculate a simple spherical problem with a uniformly heating source. The results will be compared with the one gotten from CAVEAT. If the result came from the CAVEAT is not satisfied, a modification to the Godunov technique is certainly needed before making use of CAVEAT in the presence of strong thermal sources.

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