One-dimensional Kapitza conductance: Comparison of the phonon mismatch theory with computer experiments

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We present the analog of the Khalatnikov theory for the Kapitza conductance h_K at the boundary between two dissimilar classical one-dimensional harmonic chains of atoms. We then perform steady-state molecular-dynamics computer experiments to determine h_K directly. The phonon mismatch theory gives only order-of-magnitude agreement with the computer experiments. Preliminary calculations indicate that anharmonicity increases the Kapitza conductance.

I. INTRODUCTION

In 1941, while performing experiments on liquid helium II, Kapitza[1] observed that a finite-temperature discontinuity appears between liquid helium and a metal when a heat flux is maintained across the interface. This temperature discontinuity is the result of an interfacial thermal resistance now called the Kapitza resistance R_K. Although the name "Kapitza resistance" originally applied only to liquid helium-solid interfaces, its use to describe any thermal boundary resistance is generally accepted.

Theoretical explanations of the Kapitza conductance $h_K (h_K \equiv R_K^{-1})$ have failed whenever a quantum liquid or quantum solid is present on one side of the interface,[2] indicating that for these cases the fundamental mechanisms are not well understood. Even for classical systems, however, there are reasons for doubting the usual theoretical explanations, as will be pointed out in Secs. II and III. We have therefore undertaken a study of the Kapitza conductance for simple systems by using molecular-dynamics computer experiments.[3] (By molecular dynamics we mean a computer experiment in which the behavior of a system of particles is analyzed by numerical integration of the equations of motion.) Using molecular dynamics, one may vary the particle masses, the lattice constants, the interatomic forces, and the temperatures of and the interactions with thermal reservoirs. Hence, one may determine which properties of the lattices most influence the Kapitza conductance. Moreover, one may study how the anharmonic terms in the interactions (which are essential to the theories of the thermal conductivity and thermal expansion of solids) affect the magnitude of h_K; these terms render analytic approaches relatively intractable. It is possible that the large anharmonicity of quantum systems, not their quantum nature per se, is the element missing from previous theoretical work.

There are a number of disadvantages in using molecular dynamics. One of these is the cost in terms of computer time. A typical computer calculation for a 35-particle lattice and for 10^5 fourth-order Runge-Kutta integration steps takes approximately 50 min on an IBM 360/65. Straightforward calculations of h_K for two-dimensional lattices might prove to be prohibitively expensive. Therefore, the present study is restricted to one-dimensional systems, and one must be cautious about extrapolating the results. Moreover, the calculations are necessarily classical and therefore cannot generate any intrinsically quantum-mechanical effects.

It is clear that our results cannot be applied directly to any real systems. The major objective of the present study is to compare the h_K calculated from computer experiments with that from the Khalatnikov acoustic mismatch theory which we extend to shorter wavelengths (hence phonon mismatch theory). We find only order-of-magnitude agreement between these two approaches.

A short review of the previous theoretical work on the Kapitza conductance problem is presented in Sec. II. Section III contains a presentation of the Khalatnikov (phonon) mismatch theory for the one-dimensional case. In Sec. IV, the direct steady-state molecular-dynamics (SSMD) calculations of h_K for various lattices is presented. Sec. V contains a summary and discussion.

II. REVIEW OF THEORETICAL WORK ON h_K

Although a sizable amount of theoretical work has been done in the last 25 years, no satisfactory treatment of the Kapitza problem has been given; theoretical values of h_K are often smaller than experimental ones by an order of magnitude or

more.[4] Khalatnikov[5] and, independently, Mazo[6] developed an acoustic mismatch theory to describe the Kapitza conductance for the specific case of a solid-liquid helium interface. Although the Khalatnikov theory appears to be satisfactory for interfaces between classical solids and classical liquids, the theory fails whenever a quantum solid or quantum liquid is present, except at temperatures below 0.1°K.[2,4]

Early in the history of this problem, Little[7] pointed out a serious difficulty with the Khalatnikov theory—that when the two materials become identical, so there is no interface, the Khalatnikov theory does not predict an infinite Kapitza conductance. However, he provided no alternative to the Khalatnikov theory.

Simons[8] and, independently, Visscher[9] subsequently modified the Khalatnikov theory to include, on each side of the interface, phonon distribution functions which have two components. The first is the Bose-Einstein equilibrium distribution assumed by Khalatnikov which can support no heat current (we shall call this assumption the Khalatnikov ansatz). The second term is a nonequilibrium distribution which is responsible for the heat current. Although the resulting correction to the Kapitza conductance is in the right direction to lessen the discrepancy with experiment, its magnitude is generally inadequate.[8,9] This modified Khalatnikov theory, however, does have the desirable property that if the materials on each side of the interface become identical, then h_K does indeed diverge. We will apply it in the next section to the one-dimensional problem.

Haug and Weiss[10] and Peterson and Anderson[11] have attempted to explain the experimental values for h_K at a ^{4}He-solid interface in the $0.1 \lesssim T \lesssim 1.0$ °K regime by taking into account the phonon absorption in the solid as caused, for instance, by scattering off surface dislocations. Vuorio[12] has observed that these theories, which attempt to account for phonon attenuation, suffer from three important defects. First, they do not satisfy the principle of detailed balance in thermal equilibrium. Second, the complex wave vector introduces dissipation into the system, but the question of where the energy goes and how that affects the transmission is neglected. Third, a complex wave vector does not properly describe the attenuation (due to scattering) of a phonon. Such an approach may be used for electromagnetic radiation in a metal, where the scattering is delocalized, but not for phonons of thermal energies where the scattering centers are well separated compared to the phonon wavelength.

Other attempts on the Kapitza conductance problem have been initiated within the framework of transport theory. Budd and Vannimenus[13] used a simple Boltzmann equation approach to provide a phenomenological description of thermal transport across a metal-insulator interface, using this to calculate the spatial variation of the temperature. Erdös and Haley also have used a simplified Boltzmann equation in a related study.[14] Later, Saslow formulated the Kapitza conductance problem within the framework of transport theory in a more general and rigorous manner, utilizing the surface solutions of the Boltzmann equation to match the boundary conditions at the interface.[15,16] Unfortunately, the complexity of the transport theory approach has prevented its application in specific calculations. It should be noted that acoustic mismatch and related theories omit the surface solutions of the Boltzmann equation (which are included in the transport theory approaches), thus neglecting volume scattering in the vicinity of the interface.

The transmission coefficient at the interface is of fundamental importance in the Khalatnikov theory of the Kapitza conductance, and an adequate explanation for its magnitude, at least when a quantum system is present, does not exist. It is interesting to note that, in at least one case, a simple classical theory has had unusual success. Sluckin[17] proposed a classical billiard ball coupling across the interface as a model for the energy transport mechanism. The resulting transmission coefficients for interfaces between liquid helium and various solids (with atomic weights between 30 and 210) agree surprisingly well with experimental results.

Although this review of previous theoretical work on the Kapitza conductance problem is by no means complete, two facts do emerge: (i) There is no general agreement on the form of the transmission coefficient α when a quantum system is present, and (ii) there is no general agreement on how to calculate h_K even if α is known (e.g., is the Khalatnikov ansatz correct, will a heat current correction suffice, is a full transport theory approach required?) Additional references may be found in the review articles by Pollack,[4] Challis,[18] and Snyder.[19] Note that we have completely ignored the h_K problem when the energy transport is mediated primarily by spin systems. This recent area of research may be traced through the references contained in Maki *et al.*[20]

III. KHALATNIKOV THEORY IN ONE DIMENSION

We shall now present the Khalatnikov theory for the classical one-dimensional case.[21] We will also include modifications to allow for the presence of a heat current. Our model is illustrated in Fig. 1.

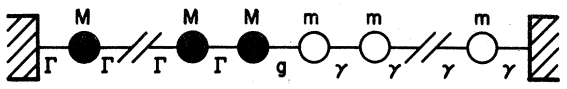

FIG. 1. One-dimensional model for the calculation of the Kapitza conductance h_K.

It consists of two semi-infinite harmonic chains, each with lattice constant a and length L, connected at the origin. The chain on the left-hand side ($n \leq 0$) is composed of atoms with mass M, nearest neighbors interacting with harmonic force constant Γ. On the right-hand side ($1 \leq n$), the chain has atoms of mass m and force constant γ. The two chains are connected by a harmonic force between atoms 0 and 1 with a force constant g. To find the transmission coefficient, one assumes a wave incident from the left, a reflected wave of amplitude R, and transmitted wave with amplitude T on the right:

$$x_n = e^{ikna} + Re^{-ikna} \quad (n \leq 0), \tag{3.1a}$$

$$x_n = Te^{iq(n-1)a} \quad (n \geq 1). \tag{3.1b}$$

Equations (3.1) give the displacement of the nth particle from equilibrium; not explicitly shown is a factor $e^{-i\omega t}$ where ω satisfies

$$\omega^2 = (2\Gamma/M)(1 - \cos ka) = (2\gamma/m)(1 - \cos qa). \tag{3.2}$$

A tedious but straightforward algebraic manipulation of the equations of motion yields

$$R = -(B^* b - g^2)/(Bb - g^2), \tag{3.3}$$

where

$$B = \Gamma(1 - e^{-ika}) - g, \tag{3.4a}$$

$$b = \gamma(1 - e^{-iqa}) - g. \tag{3.4b}$$

The ratio of transmitted power to incident power at this frequency is, for $\Gamma = \gamma = g$,

$$\alpha = 1 - |R|^2 = \frac{2 \sin ka \sin qa}{1 - \cos(ka + qa)}. \tag{3.5}$$

At the heart of the Khalatnikov theory is the assumption that

$$\dot{Q} = \sum_{k>0} n_k v_k \epsilon_k \alpha_k + \sum_{q<0} n_q v_q \epsilon_q \alpha_q, \tag{3.6}$$

for the net heat transferred per unit time across the boundary, where n_k and n_q are the number of phonons per unit volume (length in one dimension) on the left- and right-hand sides of the interface, respectively. The phonon group velocities on the left and right sides are given by v_k and v_q. The energy per phonon is given by $\epsilon_k = \hbar\omega_k$ and $\epsilon_q = \hbar\omega_q$, and $\alpha_k (= \alpha_q$ for $\omega_k = \omega_q)$ is the transmission coefficient given by (3.5). Equation (3.6) (which satisfies the Khalatnikov ansatz if the phonon distribution functions n_k and n_q are replaced by the Bose-Einstein equilibrium distribution functions $\bar{n}_k$ and $\bar{n}_q$) has a certain intuitive appeal. It is, in fact, correct if the phonon density matrix is diagonal, and forces are harmonic everywhere, allowing no inelastic scattering. In the solid-liquid situation, neither of these conditions is close to being satisfied; in the solid-solid case the forces may be nearly harmonic, but due to boundary conditions the density matrix near the interface is not expected to be diagonal. Nevertheless, the Khalatnikov ansatz does, in some situations at least, give fairly accurate results for the Kapitza conductance, as we will show in the following.

We proceed to evaluate (3.6) by splitting n_k into an even part and an odd part in k, viz.,

$$n_k = \bar{n}_k + \hat{n}_k, \tag{3.7}$$

and assuming that the even part $\bar{n}_k$ is a Bose-Einstein equilibrium distribution. (The distribution n_q is treated the same way.) The odd part $\hat{n}_k = -n_{-k}$ is entirely responsible for the heat current since in the bulk,

$$\dot{Q} = \sum_k n_k v_k \epsilon_k = 2\sum_{k>0} v_k \epsilon_k \hat{n}_k = 2\sum_{q>0} v_q \epsilon_q \hat{n}_q. \tag{3.8}$$

If we now assume that there is a small temperature difference $\Delta T = T_L - T_R$ between the two sides and note that in the high-temperature limit the phonon densities become

$$\bar{n}_k = k_B T_L / L\epsilon_k, \tag{3.9a}$$

$$\bar{n}_q = k_B T_R / L\epsilon_q, \tag{3.9b}$$

then (3.6) becomes

$$\dot{Q} = \dot{Q}_K + \tfrac{1}{2}\dot{Q}(\bar{\alpha}_L + \bar{\alpha}_R). \tag{3.10}$$

Here $\dot{Q}_K$ is the heat current in the Khalatnikov ansatz, given by

$$\dot{Q}_K = \frac{k_B \Delta T}{L} \sum_{k>0} v_k \alpha_k \tag{3.11}$$

and

$$\bar{\alpha}_L = \sum_{k>0} \hat{n}_k v_k \alpha_k \epsilon_k \Big/ \sum_{k>0} \hat{n}_k v_k \epsilon_k, \tag{3.12}$$

$$\bar{\alpha}_R = \sum_{q>0} \hat{n}_q v_q \alpha_q \epsilon_q \Big/ \sum_{q>0} \hat{n}_q v_q \epsilon_q. \tag{3.13}$$

If we now define $\bar{\alpha}$ by

$$\bar{\alpha} = \tfrac{1}{2}(\bar{\alpha}_L + \bar{\alpha}_R), \tag{3.14}$$

then

$$\dot{Q} = (1 - \bar{\alpha})^{-1}\left(\frac{k_B}{L} \sum_{k>0} v_k \alpha_k\right)\Delta T . \tag{3.15}$$

We identify the Kapitza conductance $h_K = \dot{Q}/\Delta T$ and find

$$h_K^c = (1 - \bar{\alpha})^{-1} h_K^K , \tag{3.16}$$

where the superscript c signifies that the conductance has been "corrected" to account for the heat current and where h_K^K is the conductance in the Khalatnikov ansatz given by

$$h_K^K = \frac{k_B}{2\pi} \int_0^{\omega_0} \alpha(\omega)\, d\omega . \tag{3.17}$$

Clearly if the two materials become identical, $\alpha(\omega)$ and $\bar{\alpha}$ approach unity and $h_K^c \to \infty$, meaning that a nonexistent boundary cannot support a temperature difference. In situations where the transmission coefficient is large, the factor $(1-\alpha)^{-1}$, which has been omitted from most discussions of thermal boundary resistance, becomes important.

In order to evaluate (3.12) and (3.13) one must determine an expression for $\hat{n}_k$. A natural thing would be to consider the momentum-independent relaxation time approximation, in which $\hat{n}_k$ is given by[22]

$$\hat{n}_k = -\tau v_k \frac{\partial \bar{n}_k}{\partial T} \frac{\partial T}{\partial x} \quad (\bar{n}_k \gg \hat{n}_k) , \tag{3.18}$$

where v_k is the phonon-group velocity. However, this leads to a divergent integral in the one-dimensional case. An alternate expression for $\hat{n}_k$ may be found with the drift-velocity approximation. In the drift-velocity approximation, we write the phonon distribution as

$$n_k = \{\exp[(\epsilon_k - \hbar k v_d)/k_B T] - 1\}^{-1} , \tag{3.19}$$

where v_d is the phonon drift velocity responsible for the heat current. Expanding (3.19) in the form of (3.7), one finds

$$\hat{n}_k = k_B T k \hbar v_d \epsilon_k^{-2} . \tag{3.20}$$

We have numerically evaluated $\bar{\alpha}$ by using (3.12), (3.13), (3.14), and (3.20), and h_K^K by using (3.17). The Khalatnikov and "corrected" conductances, h_K^K and h_K^c, are plotted in Fig. 2 as a function of the mass mismatch across the boundary (the values $m = 1.0 \times 10^{-22}$ g and $\gamma = 8.2556 \times 10^2$ erg/cm^2, appropriate to Ar, were used in the calculations).

IV. STEADY STATE MOLECULAR DYNAMICS (SSMD)

In this section we report calculations of the Kapitza conductance based on computer experiments which track the behavior of the lattice until steady-state behavior is achieved. The model

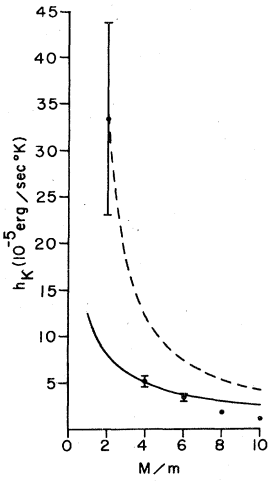

FIG. 2. Kapitza conductance versus mass ratio for harmonic lattices. The one-dimensional Khalatnikov conductance h_K^K is represented by the solid line. The "corrected" Khalatnikov conductance h_K^c is represented by the dashed line. The data points (●) represent h_K^{in} values found from SSMD calculations.

used for the calculations is essentially the same as that described by Payton *et al.*[3] The primary difference between these models is that we divide the one-dimensional lattice into two parts with different masses and (harmonic and anharmonic) forces. This is a model for two dissimilar contiguous crystals. By a mechanism to be discussed later, one end of the chain interacts with a hot thermal reservoir, the other with a cold reservoir; this results in a flow of heat through the chain which finally assumes steady-state behavior. The measured Kapitza conductance is

$$h_K = \langle \dot{Q} \rangle / \Delta T , \tag{4.1}$$

where $\dot{Q}$ is the net heat current at some point in the chain, the brackets denote a time average, and ΔT is the temperature discontinuity at the interface. We evaluate $\dot{Q}$ by keeping track of energy exchange with the thermal reservoirs.

The integration of the equations of motion of the lattice for each time step is performed by using a fourth-order Runge-Kutta integration technique. To monitor the accuracy of the integrations, the initial energy of the lattice is calculated immediately after the initial positions and velocities have been chosen. During the calculations, a record of the energy flow at each end is stored. At regular intervals, the total energy of the lattice is calculated, the net energy flow into the lattice from the reservoirs is subtracted from it, and the result is compared with the initial energy. This check of energy conservation is a measure of the accuracy of the numerical integration which, in turn, depends on the integration step size. For a lattice containing 60 particles ($m = 1.0 \times 10^{-22}$ g, $\gamma = 8.2556 \times 10^2$ erg/cm^2), for $T \leq 3$ °K, and for 10^5 time steps (we have chosen our time step size to be 2.67×10^{-14} sec, which is about 1/40 of the mini-

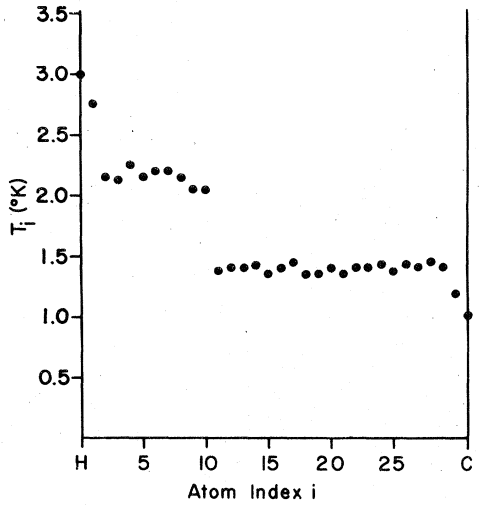

FIG. 3. Typical temperature profile after 10^5 integrations. Atoms $i=1$ through $i=10$ have mass M, and atoms $i=11$ through $i=30$ have mass m where $M/m=4$; the lattice is harmonic. The points on the abscissa labeled by H and C are plotted to show the temperatures of the hot and cold reservoirs, respectively.

mum phonon period) the error in the energy is found to be less than 0.3%.

To monitor the progress of the system toward the steady state, the temperature profile of the lattice is calculated at regular intervals, the local temperature being the time-averaged kinetic energy of the ith atom:

$$\tfrac{1}{2}k_B T_i = \tfrac{1}{2} m_i \langle v_i^2 \rangle . \tag{4.2}$$

(Our choice of the interval for the time averaging is discussed later.) A typical temperature profile is plotted in Fig. 3. In order to determine the magnitude of the temperature discontinuity ΔT, least-squares fits to straight lines are performed for the local temperatures on each side of the interface. The resulting straight lines are extrapolated to the interface and the difference between them there is called ΔT, the temperature discontinuity. Figure 3 also shows temperature jumps at the interfaces between each end of the chain and its respective reservoir (also observed by Payton *et al.*[3]). To insure that the straight-line fits contain only bulk-temperature information, atoms adjacent to the reservoir or to the interface are omitted from the analysis.

In order that the conductance is calculated when the system is in the steady state, we employ the empirical observation (noted by Payton *et al.*[3] and supported by the present work) that after 10^4 time steps the heat current into the lattice is approximately equal to the heat current out. We typically follow the behavior of the lattice through 3×10^5 time steps and then perform a statistical analysis on the information from each of the time-averaging intervals, which are chosen to be 10^4 time steps.

Because of thermal fluctuations, the value of $\langle \dot{Q}_{\rm in} \rangle$ and $\langle \dot{Q}_{\rm out} \rangle$, the time-averaged heat flow at the hot and cold ends of the lattice, are different for any finite time interval. Therefore, in order to determine the magnitude of the thermal fluctuations, two Kapitza conductances, $h_K^{\rm in}$ and $h_K^{\rm out}$, are calculated for each lattice using $\langle \dot{Q}_{\rm in} \rangle$ and $\langle \dot{Q}_{\rm out} \rangle$ in Eq. (4.1). The results are summarized in Table I, which shows a considerable increase in the precision of the conductance values in going from an average for ten intervals (each interval consists of 10^4 time steps) to an average for 30 time intervals. For all mass ratios, the values of $h_K^{\rm in}$ and $h_K^{\rm out}$ are approximately equal at 3×10^5 time steps; we consider this to be sufficient evidence that the system is exhibiting steady-state behavior.

As in the approach of Payton *et al.*, energy enters and leaves the lattice through impulsive collisions of the end atoms with atoms from their re-

TABLE I. Steady-state molecular-dynamics conductance values for various mass ratios and for three time durations. The values of h_K have the units 10^{-5} erg/sec °K. The lattices are harmonic.

Integrations	h_K	M/m = 2	4	6	8	10
1×10^5	$h_K^{\rm in}$	51.67±27.38	5.39±1.02	4.37±0.57	2.14±0.29	1.32±0.30
	$h_K^{\rm out}$	47.97±23.02	5.73±1.32	4.51±0.86	1.95±0.25	1.32±0.29
2×10^5	$h_K^{\rm in}$	35.58±14.23	5.08±0.71	3.68±0.40	1.94±0.19	1.20±0.23
	$h_K^{\rm out}$	33.64±12.11	5.33±0.80	3.83±0.54	1.81±0.16	1.18±0.18
3×10^5	$h_K^{\rm in}$	33.45±10.37	5.19±0.57	3.44±0.31	1.77±0.14	1.11±0.22
	$h_K^{\rm out}$	31.76± 8.89	5.32±0.58	3.50±0.38	1.73±0.12	1.17±0.18

spective thermal reservoirs. The two end atoms are each connected to a fixed wall. To couple the lattice to the reservoirs, we allow each end atom to suffer an instantaneous elastic collision with a reservoir atom whose velocity has been chosen with a Gaussian random-number generator corresponding to the reservoir temperature. Instead of periodically allowing a collision between each end atom and its reservoir (for instance, once every few time steps), collisions are attempted every time step with a probability λ of success. As would be expected from the work of Rieder *et al.*,[23] we found that the efficiency of the coupling between the thermal reservoirs and the bulk lattice is strongly dependent on λ. For example, for $\lambda = 1$ the coupling is extremely poor because the bulk-lattice atoms never have the time to respond to the rapid discontinuous velocity changes of the end atoms; the system (the lattice) is being driven (by the reservoirs) principally at frequencies far above any resonant frequency of the system. The optimum value of λ was found to be given by $\lambda^{-1} \simeq 15$ time steps; larger values of λ degraded the reservoir-lattice coupling, and smaller values of λ made $\dot{Q}$ unacceptably small. This is actually an "experimental" verification of a prediction of Ref. 23 that the heat current is maximized for the maximum frequency ω when $\lambda = \frac{1}{2}\sqrt{3}\,\omega$. Using $\omega = (\gamma/m)^{1/2}$ where $\gamma = 8.2556 \times 10^2$ erg/cm^2 and $m = 1.0 \times 10^{-22}$ g, the resulting value for λ is 2.5×10^{12} sec^{-1}. For a step size of 2.67×10^{-14} sec, this means that $\lambda^{-1} = 15.05$ time steps, which is very close to the value found "experimentally."

The kinetic temperature which we observe in our harmonic lattices changes rapidly near each reservoir and is then more or less constant until the interface is approached. The rapid temperature variations in the vicinity of the reservoirs would seem to suggest that surface solutions of the Boltzmann equation are present.[13-16] A harmonic lattice, however, has no phonon collisions and, therefore, no Boltzmann equation associated with it. It is interesting to note that random computer round-off error and errors produced by the Runge-Kutta integrations have the effect that each atom in the lattice is subjected to a very weak stochastic force which simulates collisions. A model which explicitly incorporates such a stochastic force, in the form of a reservoir at each site, has been studied by Bolsterli *et al.*[24] Note that Rieder *et al.*[23] have made an analytical study of heat flow across a one-dimensional harmonic chain, finding rapid variations in the kinetic temperatures in the vicinity of the reservoirs. In their model, collisions do occur with the reservoirs and this is sufficient to produce exponential temperature profiles at the interfaces with the reservoirs. They found, however, a peculiar temperature variation which drops (rises) as the hot (cold) reservoir is approached. Most likely this is an artifact of their model, having to do with the reservoir coupling. This reservoir coupling simulates collisions with the end atoms only on the average; the computer experiments explicitly account for the rapidly fluctuating nature of the interactions with the reservoirs, as well as their average behavior.

We now discuss our SSMD results for h_κ. For 30 time intervals and various mass ratios, $h_\kappa^{\rm in}$ is plotted in Fig. 2. The SSMD conductance $h_\kappa^{\rm in}$ for the mass ratio of 2 is, within statistical error, in agreement with h_κ^c, the conductance corrected for the heat flux. The large error bars for this mass ratio occur because of large χ^2 in the least-squares fit to the temperature profile; the values of $\langle \dot{Q}_{\rm in} \rangle$ and $\langle \dot{Q}_{\rm out} \rangle$ are equal to within 0.2%. For mass ratios of 4 and 6, however, the h_κ^κ values are in agreement with the $h_\kappa^{\rm in}$ values. For the largest mass ratios of 8 and 10, the h_κ^κ values are about twice the $h_\kappa^{\rm in}$ values. The behavior of the SSMD conductances suggests two things. First, the "corrected" conductance h_κ^c is too big at the larger mass mismatches. Second, the Khalatnikov prediction, h_κ^κ, is probably unreliable because it significantly overestimates h_κ at large mismatch; no particular significance can be attributed to the fact that the Khalatnikov values agree with the SSMD values for mass ratios of 4 and 6, because their curves must cross somewhere. Since most systems of experimental interest correspond to very large mass mismatches, our results suggest that the Khalatnikov theory may be unacceptable in these cases.

In order to check the size dependence of the SSMD conductance values for large mass ratios, we performed a second calculation of $h_\kappa^{\rm in}$ and $h_\kappa^{\rm out}$ for $M/m = 8$ with a lattice twice as large as the lattice used for the $M/m = 8$ values in Table I. The size dependence, if any, is less than the statistical error.

We have also performed some preliminary SSMD studies of the dependence of h_κ on the anharmonic coefficients in the interatomic potentials for various mass ratios. Payton *et al.*[3] wrote down the first four terms of the Taylor-series expansion of the Lennard-Jones potential as

$$V(r) = -\epsilon_0 + \tfrac{1}{2}\gamma(r - r_0)^2 - \tfrac{1}{3}\mu(r - r_0)^3 + \tfrac{1}{4}\nu(r - r_0)^4 , \tag{4.3}$$

where ϵ_0 is the potential depth, r_0 is the equilibrium separation distance, and γ, μ, and ν are given by

$$\gamma = 72\epsilon_0/r_0^2, \tag{4.4a}$$

$$\mu = 756\epsilon_0/r_0^3, \tag{4.4b}$$

$$\nu = 4452\epsilon_0/r_0^4. \tag{4.4c}$$

So far we have studied only anharmonic lattices for which the forces are the same on both sides of the interface (the only mismatch being in the masses). Preliminary calculations of the Kapitza conductance for $M/m = 4$ which include the cubic and quartic anharmonic terms are presented in Table II. The values labeled "anharmonicity = 1" employ the following potential coefficients (which are similar to those for argon):

$$\gamma = 8.2556 \times 10^2 \text{ erg/cm}^2, \tag{4.5a}$$

$$\mu = 2.2714 \times 10^{11} \text{ erg/cm}^3, \tag{4.5b}$$

$$\nu = 3.5048 \times 10^{19} \text{ erg/cm}^4. \tag{4.5c}$$

In order to study the effects of different anharmonicity we keep the same value of γ and scale μ and ν according to Eq. (4.4); i.e., if μ is changed to $n\mu$, then ν is changed to $n^2\nu$. (This corresponds to keeping ϵ_0/r_0^2 constant and decreasing r_0 to r_0/n.) We describe the resultant potential as having "anharmonicity = n." The values labeled "anharmonicity = 0" are, of course, the harmonic results for the same number of time steps. As seen in Table II, increased anharmonic strengths increase h_K above the Khalatnikov value and in the right direction (if the same holds true for laboratory systems) to lessen the disagreement with experimental results.

TABLE II. SSMD conductance values for different anharmonicities. The mass ratio is $M/m = 4$ and the values are for 10^5 integrations. The Khalatnikov value is $h_K = 5.05 \times 10^{-5}$ ergs/sec °K and the "corrected" Khalatnikov value is $h_K^c = 12.00 \times 10^{-5}$ erg/sec °K for the harmonic lattice.

Anharmonicity	h_K (10^{-5} erg/sec °K) h_K^{in}	h_K^{out}
0	5.39 ± 1.00	5.73 ± 1.30
1	5.38 ± 0.77	5.82 ± 1.15
2	11.47 ± 2.34	10.86 ± 1.94

V. SUMMARY AND DISCUSSION

In order to test the validity of the Khalatnikov ansatz, we have calculated the Kapitza conductance h_K of one-dimensional harmonic lattices for various mass ratios by several methods. First, the one-dimensional analog of the Khalatnikov acoustic mismatch theory was developed. Second, the Khalatnikov theory was modified to account for the presence of a heat current through the lattice. Third, h_K was calculated for these harmonic lattices by using steady-state molecular-dynamics computer experiments.

To be brief, the Khalatnikov ansatz is not supported by the results of our computer experiments. Note that we have treated only the case of classical systems with phonons described by classical statistics as opposed to the case of classical systems with phonons described by quantum statistics, for which experimental evidence already exists[4,25] to support the Khalatnikov ansatz. Because of the classical statistics, phonons of large wavevector make an important nonacoustic contribution to h_K, and in this way the computer experiments differ from laboratory experiments.

In addition to the studies of harmonic lattices, we have also performed preliminary SSMD calculations of h_K for anharmonic lattices. The calculated conductances are larger than those for harmonic lattices and are in the right direction (although insufficient in magnitude) to lessen the disagreement with experimental results. We are presently conducting more detailed studies of the effects of anharmonicity.

To conclude, it cannot be overemphasized that the present results constitute the first Kapitza conductance experiments (computer or otherwise) on a "clean" system. It is clear that the phonon mismatch theory for this system (where the phonon transmission coefficient is well understood) does not agree with the computer experiments. However, it does give better than order-of-magnitude agreement for the cases we have studied so far. (Recall that we have not yet studied the effect of force-constant mismatch.) It may be that the present disagreement between the acoustic mismatch theory and laboratory experiments arises not so much from the Khalatnikov ansatz as from the fact that the phonon transmission coefficient is poorly understood.[26-28]

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