Thermal conductivity and thermodynamics of phonons for an exactly soluble model of disorder

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We calculate the exact thermal conductivity and the heat capacity of an insulator for which the lattice dynamics are given by a phonon gas in the presence of frozen-in disorder, in the special case of the "backward-scattering" model of impurity scattering.

The thermal conductivity of an insulator is difficult to calculate theoretically; transport theory applied to phonons is notoriously inexact and inconclusive. Recently, however, the Kubo-type formulas for such systems have been formulated.[1] Nevertheless, these formulas are rather complicated and in general require summation of an infinite number of diagrams, so that in the process of evaluating them a certain number of simplifications and approximations have been found useful or necessary.[1] The effects of scattering on the thermodynamics properties are also of physical interest. One would like to know, in general, how the changes in thermodynamics properties due to scattering effects correlate with the transport properties.

In this paper we examine an extremely simple and exactly solvable "backward-scattering model", in which stabilizing anharmonicities are included. For this model, we can obtain the one- and two-body Green functions without any approximation. A similar model has been used successfully in the study of classical transport[2] and in the electron gas.[3] We believe this to be the first application to phonons. The thermal conductivity and specific heat (or arbitrary other thermodynamic functions) are found exactly, in terms of normalized distribution functions $P_{\mathbf{q}}(v_{\mathbf{q}})$ of the random scattering matrix elements $v_{\mathbf{q}}$. The result for the latter is

$$c(T)=k_B\beta^2(2\mathrm{Vol})^{-1}\times\sum_{\mathbf{q},\sigma}\int dv_{\mathbf{q}}P_{\mathbf{q}}(v_{\mathbf{q}})\times\{\Omega_\sigma(v_{\mathbf{q}})/[2\sinh(\beta\Omega_\sigma(v_{\mathbf{q}})/2)]\}^2 , \tag{1}$$

where $\beta=1/k_BT$, $\hbar=1$, $\sigma=\pm$, and

$$\Omega_+(v_{\mathbf{q}})\equiv\begin{cases}\omega_{\mathbf{q}}\sqrt{2(2|v_{\mathbf{q}}|-1)}, & v_{\mathbf{q}}<-1/2\\ \omega_{\mathbf{q}}\sqrt{1+2v_{\mathbf{q}}}, & -1/2<v_{\mathbf{q}}<1/2\\ 2\omega_{\mathbf{q}}\sqrt{v_{\mathbf{q}}}, & v_{\mathbf{q}}>1/2 ,\end{cases} \tag{2}$$

$$\Omega_-(v_{\mathbf{q}})\equiv\begin{cases}2\omega_{\mathbf{q}}\sqrt{|v_{\mathbf{q}}|}, & v_{\mathbf{q}}<-1/2\\ \omega_{\mathbf{q}}\sqrt{1-2v_{\mathbf{q}}}, & -1/2<v_{\mathbf{q}}<1/2\\ \omega_{\mathbf{q}}\sqrt{2(2v_{\mathbf{q}}-1)}, & v_{\mathbf{q}}>1/2 .\end{cases} \tag{3}$$

Here $\omega_{\mathbf{q}}$ is the frequency of the $\mathbf{q}$th normal mode, in the absence of disorder. For perfect crystals, $P_{\mathbf{q}}(v_{\mathbf{q}})$ approaches a delta function $\delta(v_{\mathbf{q}})$, and (1) reduces to the textbook formula for the lattice specific heat. The specific heat associated with disorder is $c(T)-c_0(T)$, where

$$c_0(T)=k_B\beta^2(\mathrm{Vol})^{-1}\sum_{\mathbf{q}}[\omega_{\mathbf{q}}/2\sinh(\beta\omega_{\mathbf{q}}/2)]^2 .$$

The *high-temperature* limit of $c(t)$ is obtainable in a straightforward manner. In the limit $\beta\to0$, $[\omega_{\mathbf{q}}/2\sinh(\beta\omega_{\mathbf{q}}/2)]^2\to\beta^{-2}$, with $\int dv\,P(v)\equiv1$ independent of the choice of $P(v)$ and the sum over $\mathbf{q}$ restricted to the first Brillouin zone, Eq. (1) yields the usual Dulong-Petit value of k_B per site in this limit.

To analyze the *low-temperature* behavior, more information concerning $P_{\mathbf{q}}(v_{\mathbf{q}})$ is required, it is convenient to examine P near the two critical points, $|v|=0$ and $|v|=\frac{1}{2}$. For $|v|$ near 0, the normal modes are close to those of a perfect crystal, so that the resulting contribution in three-dimensions is $\propto T^3$, the Debye law. But if there is a finite probability that $|v|\geq\frac{1}{2}$, we find that under fairly general circumstances it is this region that dominates the low-temperature specific heat.

For suppose $P(v)\approx A(2|v|-1)^{-\gamma}$, independent of $\mathbf{q}$, in the neighborhood of $|v|\approx\frac{1}{2}$. (The exponent γ has to be <1 in order for P to be integrable). With this *ansatz* it is a matter of some simple algebra to evaluate Eq. (1) in the low-temperature limit, and obtain $c(T)\propto AT^{2(1-\gamma)}$. For *any* $-1<\gamma<1$ this contribution dominates over the T^3 contribution from the region $|v|\approx0$. A particular choice, $\gamma=\frac{1}{2}$, yields a linear specific heat at low temperature, in conformity with experimental evidence covering a wide variety of glasses.[4] Thus, it appears that strong random-scattering matrix elements, $|v|>\frac{1}{2}$, are somehow related to the thermodynamics properties of glasses. We shall see why and how this occurs in more detail, below.

For the configurationally averaged thermal conductivity $\langle\kappa\rangle$ we find a somewhat similar-looking, yet fundamentally different, result:

$$\langle\kappa\rangle=k_B\beta^2(2\pi/3)(\mathrm{Vol})^{-1}\sum_{\mathbf{q}\neq0}P_{\mathbf{q}}(0)\omega_{\mathbf{q}}\times\{s_{\mathbf{q}}/[2\sinh(\beta\omega_{\mathbf{q}}/2)]\}^2 , \tag{4}$$

where $s_{\mathbf{q}}=\partial\omega_{\mathbf{q}}/\partial_{\mathbf{q}}$ is the sound velocity. The shape of

$P_{\mathbf{q}}(v_{\mathbf{q}})$ at $|v_{\mathbf{q}}|\neq 0$ is irrelevant to the value of κ. The formula (4) takes on a more conventional look if we identify $P_{\mathbf{q}}(0)$ with the lifetime $\tau_{\mathbf{q}}$.[5] In the glass phase, $P_{\mathbf{q}}(v_{\mathbf{q}})=0$ for $|v_{\mathbf{q}}|<\frac{1}{2}$; Eq. (4) predicts $\langle\kappa\rangle=0$. While it is true that amorphous solids have a far lower thermal conductivity than crystals, and this result goes in the right direction, it is truly extreme and is an artifact of the model.

The significance of the critical points at $|v_{\mathbf{q}}|=0$ and $\frac{1}{2}$ can be understood as follows. For *any* $|v_{\mathbf{q}}|>0$ the degeneracy between standing waves $\propto \sin(\mathbf{q}\cdot\mathbf{r})$ and $\propto\cos(\mathbf{q}\cdot\mathbf{r})$ is lifted. Traveling wave packets, which transport energy coherently, can be constructed only if these waves are degenerate. Therefore, the (configurationally averaged) thermal conductivity must come about entirely from the unperturbed fraction of normal modes, those for which $|v_{\mathbf{q}}|=0$. This explains the proportionality of $\langle\kappa\rangle$ to $P_{\mathbf{q}}(v_{\mathbf{q}}=0)$ found in Eq. (4).

The model and its motivation are described as follows. In any solid, the distribution of defects (vacancies, interstitials, foreign atoms, broken bonds, etc.) scatters plane-wave normal modes $\mathbf{k}$ into $\mathbf{k}'$, with matrix elements $M_{\mathbf{k},\mathbf{k}'}\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}$. The $M_{\mathbf{k},\mathbf{k}'}$ are governed by the nature, and spatial distribution, of the defects. Although a number of approximate theories such as the coherent potential approximation have been developed to obtain the thermal properties of defective solids by averaging over the nature, and spatial distribution, of the defects, these methods have proved incapable of yielding the delicate phase relationships among eigenstates needed to evaluate the Kubo formulas.

Now, the principal contributions in thermal transport come from the transmission and reflection coefficient of each plane-wave normal mode. Our simplified model assumes, essentially, that such coefficients may be treated as independent random variables. Specifically, we consider just the one backscattering matrix element $M_{\mathbf{k},-\mathbf{k}}\sqrt{\omega_{\mathbf{k}}\omega_{-\mathbf{k}}}\equiv v_{\mathbf{k}}\omega_{\mathbf{k}}$ with the random matrix quantity $v_{\mathbf{k}}$ governed by a statistical distribution function $P_{\mathbf{k}}(v_{\mathbf{k}})$. Because of the possibility that some $|v_{\mathbf{k}}|$ is too large, such that the normal modes $\mathbf{k}$ and $-\mathbf{k}$ become overcoupled and the renormalized frequency becomes complex, we introduce an additional *quartic* term into the model. The quartic term comes with a very small coefficient (compatible with a small Grüneisen constant). Therefore, if $|v_{\mathbf{k}}|$ is small, the quartic term has no effect but when $|v_{\mathbf{k}}|$ is sufficiently large that the modes become overcoupled, the quartic term allows a new equilibrium state to be achieved. Either way the thermodynamic and transport properties can be computed exactly for arbitrary values of the $v_{\mathbf{k}}$'s and the results averaged over the $P_{\mathbf{k}}(v_{\mathbf{k}})$'s. This is precisely what we now do. Because the procedure may be unfamiliar to those readers who are most concerned with the properties of glassy materials, we show all the steps in the calculations.

The derivation now follows, and is quite straightforward. The model Hamiltonian is $H=H_0+H_1+H_2$ where,

$$H_0=\sum_{k_z>0}(\omega_{\mathbf{k}}/2)[-P_{\mathbf{k}}P_{-\mathbf{k}}+Q_{\mathbf{k}}Q_{-\mathbf{k}}]\ , \tag{5}$$

$$H_1=\sum_{k_z>0}\omega_{\mathbf{k}}v_{\mathbf{k}}[Q_{\mathbf{k}}^2+Q_{-\mathbf{k}}^2]\ , \tag{6}$$

$$H_2=\xi\sum_{k_z>0}\omega_{\mathbf{k}}Q_{\mathbf{k}}^2Q_{-\mathbf{k}}^2\ , \tag{7}$$

and $P_{\mathbf{k}}\equiv a_{-\mathbf{k}}-a_{\mathbf{k}}^\dagger$ and $Q_{\mathbf{k}}\equiv a_{-\mathbf{k}}+a_{\mathbf{k}}^\dagger$. The $v_{\mathbf{k}}$ are independent random potentials defined for half the $\mathbf{k}$'s. As H is hermitean, $v_{\mathbf{k}}^*=v_{-\mathbf{k}}$ defines $v_{\mathbf{k}}$ over the remaining half. We will take $v_{\mathbf{k}}$ as real. The quartic term in the Hamiltonian has been added to insure stability when $|v_{\mathbf{q}}|>\frac{1}{2}$. The anharmonic parameter ξ will be taken to be arbitrarily small or even zero, at the end of the calculation. For values of $|v_{\mathbf{q}}|<\frac{1}{2}$, the anharmonic term is just a irrelevant perturbation and the limit $\xi\to 0$ can be taken safely, leaving H as a quadratic form. However, when $|v_{\mathbf{q}}|>\frac{1}{2}$, the anharmonic term proves crucial by shifting the position of each normal mode to a new, random, equilibrium position at distance of $O(1/\sqrt{\xi})$.

The "glassy phase" in the present model requires not just $|v_{\mathbf{q}}|\neq 0$, but $|v_{\mathbf{q}}|>\frac{1}{2}$. Equations (2) and (3) reflect the profound change in the spectrum as $|v_{\mathbf{q}}|$ passes through this critical point. At the critical point, one set of normal modes softens critically. Beyond it, there is found a symmetry breaking in each normal mode, and *disorder* becomes *frozen-in* at random in the amount $|f_{\mathbf{q}}|\propto 1/\sqrt{\xi}$.

Let us recast the Hamiltonian in a useful form. First, rewrite H in terms of the bare operators $\{a_{\mathbf{k}}\}$:

$$\begin{aligned}H=\sum_{k_z>0}\omega_{\mathbf{k}}\{&a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}}+1)\\&+(1/2)v_{\mathbf{k}}[(a_{\mathbf{k}}^\dagger+a_{-\mathbf{k}})^2+(a_{-\mathbf{k}}^\dagger+a_{\mathbf{k}})^2]\\&+\xi(a_{\mathbf{k}}^\dagger+a_{-\mathbf{k}})^2(a_{-\mathbf{k}}^\dagger+a_{\mathbf{k}})^2\}\ .\end{aligned} \tag{8}$$

Now perform a rotation: $a_{\mathbf{k}}=(1/\sqrt{2})(b_{\mathbf{k}}+b_{-\mathbf{k}})$ and $a_{-\mathbf{k}}=(1/\sqrt{2})(b_{\mathbf{k}}-b_{-\mathbf{k}})$. The Hamiltonian becomes

$$\begin{aligned}H=\sum_{k_z>0}\omega_{\mathbf{k}}\{&b_{\mathbf{k}}^\dagger b_{\mathbf{k}}+b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}+1\\&+(1/2)v_{\mathbf{k}}[(b_{\mathbf{k}}+b_{\mathbf{k}}^\dagger)^2+(b_{-\mathbf{k}}+b_{-\mathbf{k}}^\dagger)^2]\\&+(\xi/4)[(b_{\mathbf{k}}+b_{\mathbf{k}}^\dagger)^2-(b_{-\mathbf{k}}+b_{-\mathbf{k}}^\dagger)^2]^2\}\ .\end{aligned} \tag{9}$$

Now define $Q'_{\mathbf{k}}=(b_{\mathbf{k}}+b_{\mathbf{k}}^\dagger)/\sqrt{2}$; $P'_{\mathbf{k}}=(-i/\sqrt{2})(b_{\mathbf{k}}-b_{\mathbf{k}}^\dagger)$. In terms of these, H becomes

$$\begin{aligned}H=\sum_{k_z>0}\omega_{\mathbf{k}}\{&(1/2)P_{\mathbf{k}}'^2+(1/2)(1+2v_{\mathbf{k}})Q_{\mathbf{k}}'^2\\&+(1/2)(1-2v_{\mathbf{k}})P'^2_{-\mathbf{k}}+(1/2)Q'^2_{-\mathbf{k}}\\&+\xi[Q_{\mathbf{k}}'^2+P'^2_{-\mathbf{k}}]^2\}\ .\end{aligned} \tag{10}$$

Now interchange P and Q in the negative $\mathbf{k}$ sector: $P'_{-\mathbf{k}}\to -Q'_{-\mathbf{k}}$; $Q'_{-\mathbf{k}}\to P'_{-\mathbf{k}}$ to restore symmetry. The Hamiltonian becomes

$$\begin{aligned}H=\sum_{k_z>0}\omega_{\mathbf{k}}\{&(1/2)P_{\mathbf{k}}'^2+(1/2)(1+2v_{\mathbf{k}})Q_{\mathbf{k}}'^2\\&+(1/2)P'^2_{-\mathbf{k}}+(1/2)(1-2v_{\mathbf{k}})Q'^2_{-\mathbf{k}}\\&+\xi[Q_{\mathbf{k}}'^2+Q'^2_{-\mathbf{k}}]^2\}\ .\end{aligned} \tag{11}$$

Following Ref. 4, we perform the symmetry-breaking transformation $Q'_k \to Q'_k + f_k$ and $Q'_{-k} \to Q'_k + f_{-k}$. This introduces a number of new contributions to H: (a) constant terms,

$$(1/2)\sum_{k_z>0}\omega_k\{(1+2v_k)f_k^2+(1-2v_k)f_{-k}^2 + 2\xi(f_k^4+f_{-k}^4+2f_k^2f_{-k})\}\ , \quad (12)$$

(b) linear terms,

$$(1/2)\sum_{k_z>0}\omega_k\{[2(1+2v_k)f_k+8\xi f_k f_{-k}^2]Q'_k + [2(1-2v_k)f_{-k}+8\xi f_{-k}f_k^2]Q'_{-k}\}\ , \quad (13)$$

(c) quadratic terms,

$$(1/2)\sum_{k_z>0}\omega_k\{[1+2v_k+12\xi f_k^2+4\xi f_{-k}^2]Q_k'^2 + [1-2v_k+12\xi f_{-k}^2+4\xi f_k^2]Q_{-k}'^2 + 16 f_k f_{-k}Q'_kQ'_{-k}\}\ , \quad (14)$$

and (d) cubic terms;

$$(1/2)\sum_{k_z>0}\omega_k\{8\xi f_kQ_k'^3+8\xi f_{-k}Q_{-k}'^3+8\xi f_kQ'_kQ_{-k}'^2 + 8\xi f_{-k}Q'_{-k}Q_k'^2\}\ , \quad (15)$$

with only the quartic terms remained unaffected.

We determine the $\{f_k, f_{-k}\}$ by the stability requirement that all linear terms vanish. This leads to

$$[2(1+2v_k)+8\xi f_k^2+8\xi f_{-k}^2]f_k=0\ , \quad (16)$$

$$[2(1-2v_k)+8\xi f_{-k}^2+8\xi f_k^2]f_{-k}=0\ . \quad (17)$$

(I) For $-\frac{1}{2}<v_k<\frac{1}{2}$, the only solution is $f_k=0=f_{-k}$, (II) for $v_k<-\frac{1}{2}$, we have $f_{-k}=0$ and $f_k=\sqrt{-(1+2v_k)/4\xi}$, and (III) for $v_k>\frac{1}{2}$, we have $f_k=0$ and $f_{-k}=\sqrt{(2v_k-1)/4\xi}$.

Case I: $-1/2<v_k<1/2$

Since all f are zero, the Hamiltonian reduces to

$$H=\sum_{k_z>0}\omega_k\{(1/2)P_k'^2+(1/2)(1+2v_k)Q_k'^2 + (1/2)P_{-k}'^2+(1/2)(1-2v_k)Q_{-k}'^2\}\ , \quad (18)$$

which is easily diagonalized by a contraction-expansion transformation: $P'_k \to \lambda_k p_k$; $Q'_k \to \lambda_k^{-1}q_k$. Similarly for P'_{-k}, Q'_{-k}. The Hamiltonian becomes

$$H=\sum_{k_z>0}(1/2)\omega_k[\lambda_k^2p_k^2+(1/\lambda_k^2)(1+2v_k)q_k^2 + \lambda_{-k}^2p_{-k}^2+(1/\lambda_{-k}^2)(1-2v_k)q_{-k}^2]\ . \quad (19)$$

We choose $\lambda_k^2=\sqrt{1+2v_k}$ and $\lambda_{-k}^2=\sqrt{1-2v_k}$ and the Hamiltonian becomes

$$H=\sum_{k_z>0}\{(1/2)\omega_k\sqrt{1+2v_k}(p_k^2+q_k^2) + (1/2)\omega_k\sqrt{1-2v_k}(p_{-k}^2+q_{-k}^2)\}\ . \quad (20)$$

Finally, if we define $q_k=(1/\sqrt{2})(\alpha_k+\alpha_k^\dagger)$ and $p_k=(-i/\sqrt{2})(\alpha_k-\alpha_k^\dagger)$, then H takes the form

$$H=\sum_{k_z>0}\omega_k\{\sqrt{1+2v_k}\alpha_k\alpha_k^\dagger+\sqrt{1-2v_k}\alpha_{-k}^\dagger\alpha_{-k} + (1/2)(\sqrt{1+2v_k}+\sqrt{1-2v_k})\}\ . \quad (21)$$

Case II: $v_k<-1/2$

In this case $f_{-k}=0$ and $f_k=\sqrt{-(1+2v_k)/4\xi}$. After inserting these into Eqs. (12)–(15) and in the limit $\xi\to 0$, the Hamiltonian becomes

$$H=\sum_{k_z>0}\omega_k\{-(1/16\xi)(1-2|v_k|)^2+(1/2)[P_k'^2+P_{-k}'^2+2(2|v_k|-1)Q_k'^2+8|v_k|Q_{-k}'^2]\}\ . \quad (22)$$

As in case I, we perform a contraction-expansion transformation, getting $\lambda_k^2=\sqrt{2(2|v_k|-1)}$ and $\lambda_{-k}^2=2\sqrt{|v_k|}$. The Hamiltonian now reads

$$H=\sum_{k_z>0}\omega_k\{-(1/16\xi)(1-2|v_k|)^2 + (1/2)\sqrt{2(2|v_k|-1)}(p_k^2+q_k^2) + \sqrt{|v_k|}(p_{-k}^2+q_{-k}^2)\}\ . \quad (23)$$

In terms of the diagonal operators $\{\alpha_k\}$, H takes the form

$$H=\sum_{k_z>0}\omega_k\{\sqrt{2(2|v_k|-1)}(\alpha_k^\dagger\alpha_k+1/2) + 2\sqrt{|v_k|}(\alpha_{-k}^\dagger\alpha_{-k}+1/2) - (1/16\xi)(2|v_k|-1)^2\}\ . \quad (24)$$

Case III: $v_k>\frac{1}{2}$

Following an analogous procedure to that of case II, we get

$$H=\sum_{k_z>0}\omega_{\mathbf{k}}\{2\sqrt{v_{\mathbf{k}}}(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+1/2)+\sqrt{2(2v_{\mathbf{k}}-1)}(\alpha_{-\mathbf{k}}^{\dagger}\alpha_{-\mathbf{k}}+1/2)-(1/16\xi)(2v_{\mathbf{k}}-1)^2\}\ . \tag{25}$$

In summary, omitting the constant term, the dynamic portion of the Hamiltonian is

$$H=\sum_{k_z>0}[\Omega_+(v_{\mathbf{k}})\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+\Omega_-(v_{\mathbf{k}})\alpha_{-\mathbf{k}}^{\dagger}\alpha_{-\mathbf{k}}]\ , \tag{26}$$

where $\Omega_+(v_{\mathbf{k}})$ and $\Omega_-(v_{\mathbf{k}})$ were defined in (2). Equation (1) follows directly from Eq. (26) and from $c(T)=(\mathrm{Vol})^{-1}(d\langle H\rangle/dT)$ where $\langle H\rangle$ is the total internal energy averaged over the (random) v's.

For the thermal conductivity we start from the Kubo formula for phonons:[1]

$$\kappa=\frac{k_B\beta}{3\mathrm{Vol}}\sum_{\mathbf{k}\neq 0}\sum_{\mathbf{q}\neq 0}\mathbf{s}_{\mathbf{k}}\cdot\mathbf{s}_{\mathbf{q}}\omega_{\mathbf{k}}\omega_{\mathbf{q}}\int_0^{\infty}dt\int_0^{\beta}d\lambda\langle n_{\mathbf{k}}(0)n_{\mathbf{q}}(t+i\lambda)\rangle\ , \tag{27}$$

where $n_{\mathbf{k}}\equiv a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$ and $\langle\cdots\rangle$ indicate both thermal and configurational averages. After some algebra, κ can be expressed as

$$\kappa=\frac{ik_B\beta}{3\mathrm{Vol}}\sum_{\mathbf{k}\neq 0}\sum_{\mathbf{q}\neq 0}\mathbf{s}_{\mathbf{k}}\cdot\mathbf{s}_{\mathbf{q}}\omega_{\mathbf{k}}\omega_{\mathbf{q}}\int_0^{\infty}dt\,t\langle[n_{\mathbf{k}}(t),n_{\mathbf{q}}(0)]\rangle\ . \tag{28}$$

For the backward-scattering model, it is convenient to rewrite Eq. (28) as

$$\kappa=\frac{ik_B\beta}{3\mathrm{Vol}}\sum_{k_Z,q_Z>0}s_{\mathbf{k}}\cdot s_{\mathbf{q}}\omega_{\mathbf{k}}\omega_{\mathbf{q}}\int_0^{\infty}dt\,t\langle[n_{\mathbf{k}}(t)-n_{-\mathbf{k}}(t),n_{\mathbf{q}}(0)-n_{-\mathbf{q}}(0)]\rangle\ , \tag{29}$$

and after averaging over configurations,

$$\langle\kappa\rangle=\frac{ik_B\beta}{3\mathrm{Vol}}\sum_{k_Z,q_Z>0}\mathbf{s}_{\mathbf{k}}\cdot\mathbf{s}_{\mathbf{q}}\omega_{\mathbf{k}}\omega_{\mathbf{q}}\int dv_{\mathbf{q}}\int dv_{\mathbf{k}}P_{\mathbf{q}}(v_{\mathbf{q}})P_{\mathbf{k}}(v_{\mathbf{k}})\int_0^{\infty}dt\,t\langle[n_{\mathbf{k}}(t)-n_{-\mathbf{k}}(t),n_{\mathbf{q}}(0)-n_{-\mathbf{q}}(0)]\rangle\ . \tag{30}$$

We need to expand the commutator in terms of the diagonal operators $\{\alpha_{\mathbf{k}}\}$. Taking $k_Z>0$ for definiteness, the transformation that diagonalize H takes the following form:

$$a_{\mathbf{k}}=A_+\alpha_{\mathbf{k}}+A_-\alpha_{\mathbf{k}}^{\dagger}+B_+\alpha_{-\mathbf{k}}+B_-\alpha_{-\mathbf{k}}^{\dagger}\ , \tag{31}$$

$$a_{-\mathbf{k}}=A_+\alpha_{\mathbf{k}}+A_-\alpha_{\mathbf{k}}^{\dagger}-B_+\alpha_{-\mathbf{k}}-B_-\alpha_{-\mathbf{k}}^{\dagger}\ , \tag{32}$$

where

$$A_{\pm}=(1\pm\lambda_{\mathbf{k}}^2)/(2^{3/2}\lambda_{\mathbf{k}})\ , \tag{33}$$

$$B_{\pm}=i(1\pm\lambda_{-\mathbf{k}}^2)/(2^{3/2}\lambda_{-\mathbf{k}})\ . \tag{34}$$

The λ's are

$$\lambda_{\mathbf{k}}^2=\begin{cases}2\sqrt{|v_{\mathbf{k}}|} & v_{\mathbf{k}}<-1/2\ \text{(Case II)}\\ \sqrt{1+2v_{\mathbf{k}}} & |v_{\mathbf{k}}|<1/2\ \text{(Case I)}\\ \sqrt{2(2v_{\mathbf{k}}-1)} & v_{\mathbf{k}}>1/2\ \text{(Case III)}\ ,\end{cases} \tag{35}$$

$$\lambda_{-\mathbf{k}}^2=\begin{cases}\sqrt{2(2|v_{\mathbf{k}}|-1)} & v_{\mathbf{k}}<-1/2\ \text{(Case II)}\\ \sqrt{1-2v_{\mathbf{k}}} & |v_{\mathbf{k}}|<1/2\ \text{(Case I)}\\ 2\sqrt{v_{\mathbf{k}}} & v_{\mathbf{k}}>1/2\ \text{(Case III)}\ .\end{cases} \tag{36}$$

The integral over $v_{\mathbf{k}}$ can be divided into three portions: From $-\infty$ to $\frac{1}{2}$, from $\frac{1}{2}$ to $\frac{1}{2}$, and from $\frac{1}{2}$ to $+\infty$.

Case I: In the middle region, where $|v_{\mathbf{k}}|<\frac{1}{2}$ we get

$$\langle[n_{\mathbf{k}}(t)-n_{-\mathbf{k}}(t),n_{\mathbf{q}}(0)-n_{-\mathbf{q}}(0)]\rangle=\delta_{\mathbf{qk}}(i/2)[c_+(\langle\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}\rangle-\langle\alpha_{-\mathbf{k}}^{\dagger}\alpha_{-\mathbf{k}}\rangle)\sin((\Omega_+-\Omega_-)t)-c_-(1+\langle\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}\rangle+\langle\alpha_{-\mathbf{k}}^{\dagger}\alpha_{-\mathbf{k}}\rangle)\sin((\Omega_++\Omega_-)t)]\ , \tag{37}$$

where $c_{\pm}\equiv[(\lambda_{\mathbf{k}}^2\pm\lambda_{-\mathbf{k}}^2)/\lambda_{\mathbf{k}}\lambda_{-\mathbf{k}}]^2$ and $\langle\alpha_{\pm\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}\rangle=[\exp(\beta\Omega_{\pm})-1]^{-1}$.

Use of the identity $\lim_{\epsilon\to 0}\int_0^{\infty}dt\,t\exp(-\epsilon t)\sin(\omega t)=-\pi\delta'(\omega)$ reduces Eq. (30) for κ to

$$\langle\kappa\rangle=\frac{-\pi k_B\beta s_k^2}{3\mathrm{Vol}}\sum_{k_z>0}P_k(v_k=0)\{d(\langle\alpha_k^\dagger\alpha_k\rangle-\langle\alpha_{-k}^\dagger\alpha_{-k}\rangle)/dv_k\}_{v_k=0}\,. \tag{38}$$

But,

$$\{(d/dv)(\langle\alpha_k^\dagger\alpha_k\rangle-\langle\alpha_{-k}^\dagger\alpha_{-k}\rangle)\}_{v_k=0}=-2\beta\omega_k\exp[\beta\omega_k]/(\exp[\beta\omega_k]-1)^2\,, \tag{39}$$

so $\langle\kappa\rangle$ reduces to

$$\langle\kappa\rangle=\frac{2\pi k_B\beta^2}{3\mathrm{Vol}}\sum_{k_z>0}s_k^2\frac{P_k(v_k=0)\omega_k\exp[\beta\omega_k]}{(\exp[\beta\omega_k]-1)^2}\,. \tag{40}$$

Cases II and III: $|v_k|>1/2$. Here $Q'_k\to Q'_k+f_k$ and $Q'_{-k}\to Q'_{-k}+f_{-k}$, which implies, $a_k\to a_k+(1/2)(f_k+f_{-k})$ and $a_{-k}\to a_{-k}+(1/2)(f_k-f_{-k})$. With this, the number operators n_k transform as

$$n_k\to n_k+(1/2)(f_k+f_{-k})a_k^\dagger+(1/2)(f_k+f_{-k})a_k+(1/4)(f_k+f_{-k})^2\,. \tag{41}$$

We must use this transformed $n_k=a_k^\dagger a_k$ in Eq. (30). Let us examine one (four) of them, say $[n_k(t),n_q(0)]$. Clearly, $[n_k(t),n_q(0)]$ will give no contributions, since it is proportional to $\delta'(\Omega_+-\Omega_-)$. Because $v_q\neq0$, $(\Omega_+-\Omega_-)$ can only vanish at $\mathbf{q}=0$, which has no support. Also terms like $[n_k,a_q]$ are zero in thermal equilibrium, since they are linear in $\{a_k\}$, therefore, linear in $\{\alpha_k\}$. The surviving terms are of the form

$$(1/4)(f_k+f_{-k})(f_q+f_{-q})[a_k^\dagger(t),a_q^\dagger(0)]+(1/4)(f_k+f_{-k})(f_q+f_{-q})[a_k^\dagger(t),a_q(0)]$$
$$+(1/4)(f_k+f_{-k})(f_q+f_{-q})[a_k^\dagger(t),a_q^\dagger(0)]+(1/4)(f_k+f_{-k})(f_q+f_{-q})[a_k(t),a_q(0)]\,.$$

We have used the fact that the f are real. Expanding the bare operators a_k in terms of the eigenoperators set α_k, according to Eqs. (31) and (32) and using the fact that $A_\pm$ are always real, while $B_\pm$ are always imaginary we get, *after some algebra,* the following for the surviving terms:

$$(-1/2)\delta_{kq}(f_k+f_{-k})^2\{(A_++A_-)^2\sin(\Omega_+t)-(B_+-B_-)^2\sin(\Omega_-t)\}\,. \tag{42}$$

When replacing this into Eq. (30), we must evaluate the integrals

$$(-1/2)\delta_{kq}(f_k+f_{-k})^2(A_++A_-)^2\int_0^\infty dt\,t\sin(\Omega_+t)+(1/2)\delta_{kq}(f_k+f_{-k})^2(B_+-B_-)^2\int_0^\infty dt\,t\sin(\Omega_-t)\,. \tag{43}$$

Each one of these integrals is proportional to a δ', with support at $\Omega_+(v_k)=0$ and $\Omega_-(v_k)=0$. For $v_k<-\frac{1}{2}$, only Ω_+ can be zero, namely at $v_k=\frac{1}{2}$, while Ω_- cannot be zero. For $v_k>\frac{1}{2}$, the converse is true. Let us suppose, $v_k<-\frac{1}{2}$. Then, (43) reduces to

$$(-1/2)\delta_{kq}[(2|v_k|-1)/4\xi](1/4\sqrt{|v_k|})(-\pi\delta'(\Omega_+))\,, \tag{44}$$

where $\Omega_+=\omega_k\sqrt{-2(1+2v_k)}$. Then, Eq. (44) is essentially of the form $\Omega_+^2\delta'(\Omega_+)$, which vanishes identically.

Similarly, the other three terms arising from Eq. (30), after the symmetry-breaking transformation, give no contribution. For the case $v_k>1/2$, we also find no contribution.

So far we have only investigated the $\omega=0$ term conductivity in the context of the present exactly solvable model. However, it is also possible to generalize to finite ω, by inserting a factor $\exp(i\omega t)$ in Eq. (27). This allows to compute ultrasonic attenuation as a function of ω. With the argument in terms such as (44) being $(\Omega_\pm\pm\omega)$, one sees that the integrand leading to $\langle\kappa(\omega)\rangle$ ceases to vanish identically, for it now includes factors as $P_q[1/2\pm(\omega/\omega_q)^2]\omega^2$. While the present model is thus capable of being extended to the study ultrasonic attenuation, we leave such extensions for future investigation.

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[1]Ph. Choquard, Helv. Phys. Acta **36**, 415 (1963); J. M. Luttinger, Phys. Rev. **135**, A1505 (1964); B. Deo and S. N. Behera, *ibid.* **141**, 738 (1966).

[2]M. Dresden, Rev. Mod. Phys. **33**, 265 (1961); P. M. Bakshi and E. P. Gross, Ann. Phys. (N.Y.) **49**, 513 (1968); D. C. Mattis, A. M Szpilka, and H. Chen, Mod. Phys. Lett. B **3**, 215 (1989).

[3]Hua Chen and Daniel Mattis, Mod. Phys. Lett. B **5**, 309 (1991); Hua Chen, Daniel Mattis, and Sergey Rudin (unpublished).

[4]Mario Molina and Daniel Mattis, Phys. Lett. A **159**, 337 (1991).

[5]E.g., $P_q(0)\propto q^{-3}$ for the Rayleigh law.