Selective renormalisation: a new approach to universal properties of granular structures

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Abstract. In this paper we present a new theoretical approach to the problem of describing the dynamical properties of granular structures. For the first time a combination of the Lanczos method and a new selective renormalisation technique is used to determine the intermediate-wavelength properties of a microscopic model of a granular solid. The results show that mean-field theory correctly describes the ultra-long- and short-wavelength properties, but at intermediate wavelengths a solution of the full dynamical problem is required.

A key parameter that determines the dynamical properties of a granular structure is the ratio $C = C_s/C_b$ of the ultra-long-wavelength velocity of sound $C_s$ to the short-wavelength velocity $C_b$. For the first time, we present results for the sound velocity ratio $C$, obtained from a microscopic model of a disordered granular structure. When $C$ (corrected for porosity) decreases to less than approximately 90% of its bulk value $C_{b\nu}$, the density of phonon states $\rho(\omega)$ exhibits a low-frequency enhancement. This enhancement is expected to be a universal feature of weakly coupled granular structures. Detailed results are presented for $\rho(\omega)$, both in the presence and in the absence of disorder.

1. Introduction

Our interest in granular structures was originally stimulated by the existence of anomalies in the thermal properties of sintered metallic powders (Rutherford et al 1984) which arise when the dominant phonon wavelength $\lambda$ attains a typical grain size $L$. Such features are expected to be a general property of a wide variety of multi-phase systems, including polymeric glasses (Thorpe 1983), porous media and ceramics (Sayers 1980). Existing theories of granular structures, which focus either on the properties of isolated fine particles (Perenboom and Wyder 1981) or coupled rigid grains (Schwartz et al 1984) cannot readily yield a description of vibrational properties at these wavelengths. To obtain such a description, a new selective renormalisation technique (SRT) has recently been introduced (Lambert 1985).

The role of the SRT is to reduce a given microscopic description of a granular structure to manageable proportions. A microscopic model contains information about the high-energy internal degrees of freedom of the grains (perhaps as many as $10^9$ per grain) as well as the low-lying collective modes. The former correspond to short-wavelength excitations and are irrelevant when describing the longer-wavelength properties of the system. To reduce the problem, one selects a minimum length scale $\lambda_{\text{min}} < L$ (or
equivalently a maximum frequency $\omega_{\text{max}} = C_b/\lambda_{\text{min}}$ where $C_b$ is the bulk velocity of sound in an isolated grain) and then systematically eliminates the internal degrees of freedom with wavelength $\lambda < \lambda_{\text{min}}$. Starting from a microscopic dynamical matrix $\mathbf{H}$, this generates a renormalised model $\mathbf{\tilde{H}}$ in which each grain possesses only a small number of low-frequency internal modes. For the simplest class of microscopic models $\mathbf{H}$ contains only short-range inter-grain couplings. A key feature of the SRT is that the corresponding renormalised dynamical matrix $\mathbf{\tilde{H}}$ is independent of frequency $\omega$ and contains no long-range couplings. This simple form of $\mathbf{\tilde{H}}$ is in marked contrast with typical scaled Hamiltonians obtained in homogeneous systems, which invariably contain long-range, energy-dependent interactions (Lambert and Weaire 1981).

In the present paper we apply the SRT to a simple model of a granular structure, which in the absence of disorder in the grain sizes can be obtained by adding granularity to a scalar symmetric Born model. It is shown that in the weak-coupling limit there exists a low-frequency peak in the phonon density of states (DOS). We argue that such a DOS enhancement is a universal feature of granular structures. The behaviour of this peak is examined for a range of disorder and inter-grain couplings. We begin by considering a mean-field argument, which yields the elastic constants and the ultra-low-frequency response. In §3 a model dynamical matrix $\mathbf{H}$ is defined and selective renormalisation is employed to yield an expression for $\mathbf{\tilde{H}}$. This result was originally obtained by Lambert (1985) using diagrammatic techniques, which show that provided $\omega_{\text{max}}$ is large enough, long-range interactions can be neglected and $\mathbf{\tilde{H}}$ computed by treating pairs of grains in isolation. In §3 a much simpler derivation of the SRT is presented. In the original analysis (Lambert 1985) no systematic study of the effect of varying $\omega_{\text{max}}$ was carried out. In §4 we examine for the first time the variation of the low-frequency properties of $\mathbf{\tilde{H}}$ with $\omega_{\text{max}}$. In this way we are able to determine a suitable cut-off self-consistently from the requirement that the calculated low-frequency response does not change appreciably with a further increase in $\omega_{\text{max}}$. Finally the intermediate-wavelength properties of a granular structure are obtained, both with and without disorder and a comparison is made with mean-field theory.

2. A simple scaling argument

We begin by extending a symmetric Born model with isotropic nearest-neighbour interactions and one degree of freedom per atom to yield a model of granularity in $d$ dimensions. In §3 a model of a disordered system will be defined, but in the present section the discussion will be restricted to a crystalline granular structure. Each grain is represented by a ‘cube’ of $N^d$ atoms and the whole structure is formed by a periodic array of $R^d$ such grains. Nearest-neighbour atoms on the same grain are coupled by harmonic ‘springs’ of strength $\gamma$ and as indicated in figure 1 there is a coupling $\Gamma$ between all neighbouring atoms on adjacent faces of neighbouring cubes. The equation of motion for the single degree of freedom $U_n$ of atom $n$ is

$$m \ddot{U}_n = \sum_{n'} g_{nn'} (U_{n'} - U_n)$$

(2.1)

where $m$ is the atomic mass and

$$g_{nn'} = \begin{cases} \gamma & \text{if } n, n' \text{ are nearest neighbours on the same grain} \\ \Gamma & \text{if } n, n' \text{ are nearest neighbours on neighbouring grains} \\ 0 & \text{otherwise.} \end{cases}$$

(2.2)
Figure 1. A simple model of a granular structure formed by an array of cubic grains. Opposing atoms on adjacent faces of neighbouring grains $c, c'$ are connected by springs $\Gamma_{cc'}$. This coupling is the same for all atoms on a given pair of faces, but in general may be different for different pairs of cubes.

Note that the length $l$ of the bond $\Gamma$ does not enter the above equations explicitly and consequently cannot affect the frequency spectrum. The inter-grain bond length $l$ does, however, affect the ultra-long-wavelength velocity of sound. To describe this effect and the ultra-long-wavelength response of the model, we develop a simple mean-field theory.

Consider first the limit $l = a, \Gamma = \gamma$. In this case granularity disappears and as $\omega \to 0$ the allowed frequencies are given by

$$m\omega^2 = \gamma(\pi/RN)^2 \sum_{i=1}^{d} i_i^2 \quad i_i = 0, 1, \ldots$$  \hspace{1cm} (2.3)

Introducing a wave-vector of magnitude $K$ and the bulk velocity of sound $C_b$, where

$$K = (\pi/aRN) \left( \sum_{i=1}^{d} i_i^2 \right)^{1/2} \quad C_b = (\gamma/m)^{1/2}a$$  \hspace{1cm} (2.4)

yields the familiar long-wavelength result $\omega = C_b K$. More generally for $l \neq a$, equation (2.3) is unchanged, but the quantity $a$ of equation (2.4) must be replaced by the average atomic separation

$$\langle a \rangle = a + (l - a)/N$$  \hspace{1cm} (2.5)

to yield for the ultra-long-wavelength velocity of sound in the limit $\lambda \gg L$,

$$C_b' = (\gamma/m)^{1/2}\langle a \rangle.$$  \hspace{1cm} (2.6)

To obtain an expression for the ultra-long-wavelength velocity of sound when $\Gamma \neq \gamma$, consider first the weak-coupling limit $\Gamma \ll \gamma$. In this limit each grain can be regarded as completely rigid, with no internal degrees of freedom. In $d$ dimensions for cubes of side $L = Na$, the net spring constant between a pair of grains is $\tilde{\Gamma} = \Gamma N^{d-1}$. Since the mass of a cube is $M = mN^d$ and the new lattice constant is $A = N\langle a \rangle$ one obtains by comparison with equation (2.6)

$$C_g = (\tilde{\Gamma}/M)^{1/2}A = (\Gamma N/m)^{1/2}\langle a \rangle.$$  \hspace{1cm} (2.7)
Hence the ratio of the velocities of sound $C'_b$ and $C_g$ is

$$C = C'_b/C_g = (\Gamma N/\gamma)^{1/2}. \quad (2.8)$$

This result has been obtained by ignoring the internal degrees of freedom of the grains. Physically one expects that $C < 1$ whenever $\Gamma < \gamma$, which shows that equation (2.8) breaks down when

$$\Gamma > \gamma/N. \quad (2.9)$$

For a granular structure such as a sintered metallic powder, $N$ is typically $\sim 10^3$, so the above argument becomes invalid even at relatively small values of the inter-grain coupling and emphasises the need for a careful elimination of the internal modes. In the following section this is achieved via the SRT to yield a description of the dynamical properties of the system at wavelengths $\lambda \approx L$. Before proceeding to this we modify the above argument to yield an exact expression for the static properties of the granular structure and hence the ultra-long-wavelength velocity of sound $C_g$.

Instead of employing the bare coupling $\Gamma$ in equations (2.7) and (2.8) one should strictly use a renormalised coupling $\tilde{\Gamma}$, chosen to yield the correct elastic constants when the cubes are replaced by rigid grains. To obtain $\tilde{\Gamma}$, one notes that the effective spring constant of a chain of $N-1$ bonds $\gamma$ and a single bond $\Gamma$ is given by

$$r^{-1} = \Gamma^{-1} + (N-1)/\gamma$$

that is

$$\tilde{\Gamma} = \Gamma/[1 + (N-1)\Gamma/\gamma]. \quad (2.10)$$

Replacing $\Gamma$ by $\tilde{\Gamma}$ in equation (2.8) yields

$$C = \delta/[1 + \delta(1 - 1/N)]^{1/2} \quad (2.11)$$

where

$$\delta = \Gamma N/\gamma. \quad (2.12)$$

Within the present model, this result is exact for a crystalline granular structure in any dimension. An interesting feature of this result is that in the limit $N \to \infty$, $C$ is a universal function of $\delta$, independent of the grain size and the absolute strengths of the atomic couplings.

In the presence of disorder the problem is equivalent to that of computing the conductance of a random granular network of electrical resistors and except in one dimension has not been solved analytically. In one dimension, with a spread of grain sizes and inter-grain couplings one obtains

$$\tilde{\Gamma}^{-1} = \langle \Gamma^{-1} \rangle + (\langle N \rangle - 1)/\gamma. \quad (2.13)$$

Hence the mean-field expression for $C$ is again given by (2.11), but with $\delta$ replaced by

$$\delta = \langle N \rangle/\gamma \langle \Gamma^{-1} \rangle. \quad (2.14)$$

In § 4, numerical results in three dimensions are presented that suggest that the velocity-of-sound ratio is a function of the parameter

$$\delta = \langle N^d \rangle^{1/d}/\gamma \langle \Gamma^{-1} \rangle. \quad (2.15)$$

For $d > 1$, equation (2.11) ignores cross-links between the parallel chains of atoms that form the granular structure. Nevertheless the results of § 4 show that for $d = 3$ equation (2.11) is a remarkably good approximation for $C$. 

3. The selective renormalisation technique

In order to go beyond mean-field theory and to describe the response of a granular structure at wavelengths $\lambda = L$, a systematic elimination of the high frequency internal degree of freedom is needed. To achieve this using the SRT, we begin by defining a bare dynamical matrix $H$ describing the coupling between the internal modes of neighbouring grains. For convenience we write

$$H = H_0 + H_1$$

(3.1)

where $H_0$ describes a set of isolated grains and $H_1$ the effect of a non-zero coupling.

The internal modes of interest are the eigen-states of $H_0$. These are plane-wave states of the isolated grains with free-end boundary conditions. For a cube $c$ of side $L_c = a N_c$, the amplitude on atom $n = (n_x, n_y, n_z)$ of an internal mode with wave-vectors with $|K| = (\pi/L_c)(i^2 + j^2 + k^2)^{1/2}$, where $i, j, k = 0, 1, \ldots, N_c - 1$ is

$$\varphi_{(ijk)}(n) = \psi_i^c(n_x) \psi_j^c(n_y) \psi_k^c(n_z).$$

(3.2)

In equation (3.2)

$$\psi_i^c(n_x) = A_i^c \cos[(n_x - \frac{1}{2}) \pi/N_c]$$

where

$$A_i^c = \begin{cases} N_c^{-1/2} & \text{for } i = 0 \\ (2/N_c)^{1/2} & \text{for } i \neq 0. \end{cases}$$

(3.3)

In this representation the elements of $H_0$ are

$$H_{0(ijk), (i'j'k')}^c = \epsilon_{(ijk)} \delta_{ii'} \delta_{jj'} \delta_{kk'}$$

(3.4)

where the squared frequency $\epsilon_{(ijk)}$ is

$$\epsilon_{(ijk)} = 4 \gamma \left[ \sin^2(i \pi/2 N_c) + \sin^2(j \pi/2 N_c) + \sin^2(k \pi/2 N_c) \right].$$

(3.5)

For convenience we have set the atomic mass to $m = 1$.

The interaction matrix $H_1$ is obtained by summing the contributions from all pairs of grains. As an example consider the contribution from grains 0 and 1 of figure 1, with all neighbouring atoms on adjacent grains coupled by bonds of strength $\Gamma_{01}$. Writing $c, c' = 0$ or 1, this is of the form

$$H_{1(ijk), (i'j'k')}^c = (-\Gamma_{01})^{c+c'} \sum_n \varphi_{(ijk)}(n) \varphi_{(i'j'k')}^c(n')$$

(3.6)

where if $c = 0$ (1) the sum is over atoms on the right- (left-) most face of cube $c$. In this equation $n' = n$ if $c = c'$. Otherwise $n'$ and $n$ are neighbouring atoms of cells $c'$ and $c$ respectively (Lambert 1985). In view of equation (3.2) this simplifies to

$$H_{1(ijk), (i'j'k')}^c = (-1)^{c+c'} \Gamma_{01} f_{i,i'}^c \psi_i^c \psi_{i'}^c \sum_{n_y, n_z} \psi_j^c(n_y)$$

$$\times \psi_k^c(n_z) \psi_{k'}^c(n_x) \psi_{k'}^c(n_z).$$

(3.7)
where
\[ \psi^c_i = A_i \cos(i\pi/2N_c) \] (3.8)
and
\[ f_{i,j,c}^c = \left[ (-1)^{i+c} \delta_{c,0} \delta_{c,0} + (-1)^{i} \delta_{c,1} \delta_{c,1} + (-1)^{c} \delta_{c,1} \delta_{c,0} + \delta_{c,0} \delta_{c,1} \right]. \] (3.9)

We shall be interested in establishing those features of the low-frequency response that are universal properties of granular structures and to this end seek the simplest model \( H \) of coupling between internal modes. In the absence of disorder in the grain sizes the summation on the right-hand side of equation (3.7) reduces to a product of Kronecker deltas to yield
\[ H_{(ij)k_i(i'j')k'}^c = (-1)^{c+c'} \Gamma_{01} f_{i,j,i',j'}^c \psi_i^c \psi_{i'}^{c'} \delta_{jj'} \delta_{kk'}. \] (3.10)

When \( N_0 \neq N_1 \) the Kronecker deltas are broadened. In this case the summation depends on precise details of the relative positions of the cubes. To avoid these complications we shall adopt equation (3.10) as the definition of our model of couplings between internal modes and merely note that this reduces to a symmetric Born model in the absence of a spread in grain sizes. For \( c \neq c' \), equation (3.10) yields the total inter-grain coupling between a pair of cubes. For \( c = c' \) it yields the contribution to the intra-grain coupling of one cube due to the presence of the other. The total intra-grain coupling on a given cube is obtained by summing the contributions from each of its six neighbours.

Given the dynamical matrix \( H \) defined by equations (3.5) and (3.10) one can now generate a new matrix \( \tilde{H} = H_0 + \tilde{H}_1 \) by eliminating states between each pair of grains. eliminating all internal degrees of freedom with energies \( \varepsilon_{(ij)k} \gtrsim \varepsilon_{\max} \), where \( \varepsilon_{\max} = \omega \tilde{\omega}_{\max} \) and ignoring terms of order \( (\omega/\omega_{\max})^2 \) compared with unity yields the following expression for the renormalised contribution to \( \tilde{H} \) from the grains 0 and 1 (Lambert 1985):
\[ \tilde{H}_{(ij)k_i(i'j')k'}^c = H_{(ij)k_i(i'j')k'}^c \]
\[ - \sum_{c'=0} \sum_{i,j,k} H_{(ij)k_i(i'j')k'}^c \varepsilon_{i,j,k}^{-1} \tilde{H}_{(ij')k_i(i'j')k'}^{c'} \psi_i^c \psi_{i'}^{c'} \delta_{jj'} \delta_{kk'}. \] (3.11)

In this equation, the second summation is over all values of \( i', j', k' \) such that \( \varepsilon_{(ij)k_i} \gtrsim \varepsilon_{\max} \).
After iterating equation (3.11) and employing equations (3.3) and (3.6), the resulting infinite series can be summed exactly to yield (cf (3.10)),
\[ \tilde{H}_{(ij)k_i(i'j')k'}^c = (-1)^{c+c'} \tilde{\Gamma}_{01} \psi_i^c \psi_{i'}^{c'} \delta_{jj'} \delta_{kk'}. \]
where
\[ \tilde{\Gamma}_{01} = \Gamma_{01} \left( 1 + \sum_{c=0} \alpha_c \right)^{-1} \] (3.13)
with
\[ \alpha_c = \Gamma_{01} \varepsilon_c \sum_{c} (\psi_i^c)^2 / \varepsilon_{(ij)k}^c. \] (3.14)
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For a given value of \( j, k \) the restriction \( \epsilon_{(ij|k)} > \epsilon_{\text{max}} \) implies \( i' > n_{jk}^c \) where \( n_{jk}^c \) is an integer. Converting the summation to an integral yields in the limits \( 1 \ll n_{jk}^c \ll N_c \)

\[ \alpha_{c'} = \delta_{c'} \eta_{jk}^{c'} \]

where

\[ \delta_{c'} = N_c \Gamma_{01}/\gamma \]

and

\[ \eta_{jk}^{c'} = \frac{1}{2\pi^2} \left( \frac{2\pi^2}{j^2 + k^2} \right)^{1/2} \tan^{-1} \left( \frac{j^2 + k^2}{n_{jk}^{c'}} \right) \]

This completes the selective scale transformation. Comparison of equations (3.12) and (3.10) shows that the final result is obtained by discarding all internal degrees of freedom with energies \( \geq \epsilon_{\text{max}} \) and simultaneously replacing the inter-grain atomic couplings \( \tilde{\Gamma}_{cc'} \) by \( \tilde{\Gamma}_{cc}^{c'} \). In contrast with the results of § 2 which describe only the static and ultra-long-wavelength properties of the system, equation (3.12) contains the dynamical properties of the granular structure at frequencies less than \( \omega_{\text{max}} \). In the following section, standard numerical techniques are used to extract these properties from \( \tilde{H} \) and a comparison is made with the mean-field results of § 2.

4. Results

Before discussing results obtained by analysing the renormalised dynamical matrix of § 3, it is of interest to consider the following argument which yields many qualitative features of the low-frequency response. Consider first the form taken by the average DOS per grain \( \rho(\omega) \), when the grains are non-interacting. At high frequencies, where the phonon wavelength is much smaller than a typical grain size, Debye theory yields

\[ \rho(\omega) = L^3 \omega^2/2\pi^2 C_b^3 = \pi\Omega^2/2\omega_b^3 \]

with \( L^3 = (N_c a)^3 \), \( \omega_b = \pi C_b/\Lambda \) and \( \Omega = \omega/\omega_b \). At lower frequencies there is a cut-off in \( \rho(\omega) \) at \( \Omega = 1 \). In addition, for one degree of freedom per atom, there will be a \( \delta \)-function of unit weight at the origin, corresponding to the translationally invariant mode of each grain. This situation is illustrated in figure 2, which shows the average DOS per grain for a collection of isolated cubes with a uniform spread in size. For large disorder figure 2(c) shows that the high-frequency \( \rho(\omega) \) is approximated by Debye theory. At lower disorder \( \rho(\omega) \) becomes increasingly structured and in the absence of disorder is simply a sequence of \( \delta \)-functions corresponding to the isolated grain eigen-frequencies \( \epsilon_{ij}^{1/2} \). An important feature of these results is that the \( \delta \)-function at \( \omega = 0 \) is unaffected by the disorder.

In the presence of large disorder in the grain sizes there is little structure in the high-frequency DOS and consequently when the inter-grain coupling is switched on one expects this region of \( \rho(\omega) \) to be relatively unchanged. In contrast the \( \delta \)-function at the origin will spread to form a band of states. When \( \Omega \ll 1 \) Debye theory yields

\[ \rho(\omega) = \Pi \Omega^2/2C^3 \omega_b \]

where \( C \) is the velocity-of-sound ratio introduced in § 2. This is the expected shape of the low-frequency side of the band. In the weak-coupling limit where \( C \ll 1 \), the high-
Figure 2. The average density of states per grain for a collection of isolated cubes. This figure is trivially formed by averaging over the isolated cell frequencies $\epsilon_i$, of equation (3.5), with the cell sizes $N$ uniformly distributed over the interval $N(1 + \Delta L)$, with $N = 10^3$. The dimensionless frequency $\Omega = \omega/\omega_h$, with $\omega_h = \Pi C_\gamma/Na$. The region with $\Delta L(\%) = (a) 0$, (b) 20, (c) 50.

frequency side is subject to a cut-off at $\omega = C_\gamma/L$, i.e. at $\Omega = C$. Later we shall compare this picture with the DOS arising from the model of § 3 in the presence of disorder. We begin however with the results obtained for a crystalline granular structure.

For a periodic array of identical cubes, the Fourier transform of $\hat{H}$ is block diagonal. In this case the frequency spectrum can be obtained by a straightforward numerical diagonalisation and the DOS by a Brillouin zone integration. The mean-field arguments of § 2 suggest that in the absence of disorder the key parameter of interest is $\delta = N\Gamma/\gamma$. In the presence of disorder we shall examine results for different values of the parameter.

$$\delta = N/\gamma(\Gamma^{-1})$$

where

$$N = L/a = (N^3_0)^{1/3}.$$  \hspace{1cm} (4.4)

In what follows we show results for $N = 10^3$, which is the order of magnitude appropriate to a sintered metallic powder. Figure 3 shows the dispersion curves obtained in the absence of disorder for two values of $\delta$. Following the notation of equations (3.5), the internal degrees of freedom of a given isolated cell are conveniently labelled by an integer triplet $(i, j, k)$. In the absence of coupling the single $(0, 0, 0)$ state from each cell forms the $\delta$ function of unit weight at the origin of figure 2. When the coupling is switched on these states form the lowest-energy (acoustic) band of figure 3. The next band is formed from the triply degenerate $(1, 0, 0)$ modes and so on. For small $\delta$ the bands are extremely flat and as $\delta$ increases they broaden and mix. For comparison with mean-field
theory, the long-wavelength velocity of sound was extracted from the slope of the linear region of the lowest band. The results are shown as full circles in figure 4 and are in excellent agreement with equation (2.11), shown as a full curve in the figure.

The results of figures 3 and 4 were obtained with a cut-off of $\omega_{\text{max}} = 3\omega_k$, which is achieved by retaining the lowest 29 degrees of freedom per grain. Figure 5 shows how the calculated dispersion changes when this cut-off is varied. Figure 5(a) shows the

![Figure 3](image1)

**Figure 3.** Dispersion curves of dimensionless frequency $\Omega \rightarrow K$ for two values of the parameter $\delta$ (defined in equation (2.12)); the full curves show results for $\delta = 0.1$ and the broken curves correspond to $\delta = 1$.

![Figure 4](image2)

**Figure 4.** The full curve shows the mean-field equation (2.11) for the velocity-of-sound ratio $C$. The full circles show the corresponding results obtained by extracting the ultra-long-wavelength velocity of sound from the linear region of the lowest dispersion curve for various values of $\delta$. 
Figure 5. Dispersion curves along the (100) direction for δ = 1 and different numbers of retained states.

(0, 0, 0) band and figure 5(b) the (1, 0, 0) band. The chain curves show the dispersion obtained by retaining only these four states per grain, so the frequency of the lowest eliminated state is \( \omega_{\text{max}} = 2^{1/2} \omega_b \). Retaining the lowest eight states per grain (\( \omega_{\text{max}} = 2 \omega_b \)) produces a shift to the broken curves. The full curves show the dispersion obtained by retaining 63 states per grain (\( \omega_{\text{max}} = (19)^{1/2} \omega_b \)). The broken curves are almost coincident with these, which demonstrates that for the purpose of computing the response of a granular structure at frequencies \( \omega \leq \omega_b \) (i.e. \( \Omega \leq 1 \)) typically, no more than eight states per grain need be retained.

Figure 6 shows the density of states per grain \( \rho(\omega) \) for a crystalline granular structure. For \( \delta = 0 \) the grains are non-interacting and \( \rho(\omega) \) is given by figure 2(a). As \( \delta \) increases the \( \delta \)-functions spread and eventually form a continuous \( \omega^{2} \) band of states. The qualitative picture formed earlier suggests that disorder in the grain sizes will wash out much of the high-frequency structure. Of more interest is the behaviour of the low-frequency peak below \( \Omega = 1 \).

This is shown in more detail in figure 7. In this figure the broken curve is a plot of equation (4.2) and demonstrates that mean-field theory correctly predicts the low-frequency behaviour of the band.

In the presence of disorder in the grain sizes and couplings, \( \tilde{H} \) cannot readily be made block-diagonal. To obtain \( \rho(\omega) \) in this case an implementation of the Lanczos method due to Parlett and Reid (1980) was employed to diagonalise the renormalised dynamical matrix \( \tilde{H} \) of a \( 6 \times 6 \times 6 \) cubic array of grains with periodic boundary conditions. The results are shown in figure 8. In the absence of any detailed knowledge of the disorder in a typical granular structure, the following \( \Gamma \)-distribution for the grain sizes was
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Figure 6. The phonon density of states for a crystalline granular structure, comprising an array of identical cubes with identical atomic couplings across their faces (see figure 1). The inter-grain coupling $\Gamma$ is related to the dimensionless coupling constant $\delta$ by equation (2.12) or equivalently equation (4.3). The dimensionless frequency $\Omega$ is defined below equation (4.1).

Figure 7. The phonon density of states for a crystalline granular structure in the region of particular interest, $\Omega = 1$, for various values of the dimensionless coupling $\delta$. For comparison the broken curves show the mean-field prediction given by equations (4.2) and (2.11).

Figure 8. The average phonon density of states per grain for a disordered granular structure obtained by retaining eight states per grain in the renormalised dynamical matrix $\mathbf{H}$. In each of the figures there is a 50% uniform spread in the inter-grain couplings, so the parameter $\delta$ defined in equation (4.3) is related to the average inter-grain coupling $\langle \Gamma \rangle$ by equation (4.7). The parameter $\sigma^2$ is the second moment of the distribution of cell sizes in equation (4.6).
employed:

\[ P(z_c) = [(P - 1)!]^{-1/2} P^P z_c^{P-1} \exp(-Pz_c) \]

(4.5)

where \( z_c = (N_c/N)^3 \), with \( N \) given by equation (4.4). For such a distribution \( N^3 = \langle N_c^3 \rangle \) and \( \sigma^2 = \langle (z_c - 1)^2 \rangle = 1/P. \)

(4.6)

For the results of figure 8, \( N \) is fixed at \( 10^3 \), so the parameter \( \delta \) of equation (4.3) varies only with the distribution of inter-grain couplings. An immediate consequence of this is that if, as suggested by mean-field theory, the velocity-of-sound ratio \( C \) is a function of \( \delta \) only, then \( C \) will be independent of \( \sigma^2 \). For simplicity the bare intergrain couplings \( \{ \Gamma_{cc'} \} \) were chosen to have a uniform distribution of the form

\[ P(\Gamma_{cc'}) = (2\Delta(\Gamma))^{-1} \begin{cases} \text{for } (\Gamma)(1 - \Delta) < \Gamma_{cc'} < (\Gamma)(1 + \Delta) \\ 0 \text{ otherwise.} \end{cases} \]

In this case \( \langle 1/\Gamma \rangle = (2\Delta(\Gamma))^{-1} \ln(1 + \Delta)/(1 - \Delta) \). For the results of figure 8, \( \Delta \) was fixed at 0.5 which yields for the parameter \( \delta \) of equation (4.3)

\[ \delta = N(\Gamma)/(\gamma \ln 3). \]

(4.7)

It is useful to compare the results for \( \sigma^2 = \frac{1}{3} \), which corresponds to a small spread in grain sizes, with the crystalline results of figure 7. The main difference between the two sets of results is that the presence of band tails in figure 8 tends to eliminate the energy gaps at weaker values of \( \langle \Gamma \rangle \). For higher values of \( \sigma^2 \) this effect is more noticeable and at \( \sigma^2 = 1 \), other than for the weakest coupling shown, all gaps have disappeared. For comparison with the mean-field theory of § 2, a value of the velocity-of-sound ratio was obtained by performing a \( \chi^2 \) fit of equation (4.2) to the low-frequency side of the peaks in figure 8. The results are shown in figure 9, where for comparison the full curve shows a plot of equation (2.11). Despite the scatter in the data, these results suggest that \( C \) is indeed independent of \( \sigma^2 \) and that the mean-field result (2.11) is a good approximation in three dimensions.

Figure 9. Results for the velocity-of-sound ratio \( C = C_l/C \) obtained by performing a \( \chi^2 \) fit of the mean-field equation (4.2) to the low-frequency side of the peaks of figure 8. The results are shown as a function of the parameter \( \delta = (N_{\text{eff}}^3 d/\gamma 1/\Gamma) \) of equation (4.3) for \( \sigma^2 = 1 \) (○), \( \sigma^2 = \frac{1}{3} \) (□) and \( \sigma^2 = \frac{1}{5} \) (●). For comparison the full curve shows the predicted result (2.11) for a three-dimensional crystalline structure.
5. Discussion

In this paper we have argued that a low-frequency density-of-states enhancement should be a universal feature of weakly coupled granular structures. This is supported by results in three dimensions, obtained from a simple model of coupled grains, both with and without disorder. The model employed is the simplest model one can envisage that describes generic effects of granularity in any dimension. A key parameter is the velocity-of-sound ratio $C$ defined in equation (2.8). The numerical results suggest that, as a crude rule of thumb, there will be a noticeable density-of-states enhancement when $C \approx 0.9$. Velocity-of-sound measurements in sintered metallic powders (Malierpaard et al 1985) demonstrate that values as low as $C = 0.2$ are attainable and hence such effects should be measurable experimentally. For the model considered, we have noted that in the absence of disorder $C$ is a universal function of the parameter $\delta$ defined in equation (2.15). In the presence of disorder the same functional form for $C$ is satisfied exactly in one dimension and appears to hold in higher dimensions.

The present analysis suggests that by varying the degree of sintering between powder grains, enhanced thermal contact between liquid $^3$He and a sintered metallic powder may be possible. A typical experiment (Harrison 1979) to cool liquid $^3$He to sub-millikelvin temperatures consists in placing the liquid in thermal contact with an adiabatically demagnetised copper refrigerant. Thermal contact is made via blocks of sintered metallic powder which are bonded to the copper surface. In practice the lowest temperature attainable is fixed by the heat leak $Q$ into the refrigerator. This generates a temperature discontinuity $\Delta T$ at the $^3$He/sinter boundary, given by $Q = \kappa \Delta T$, where $\kappa$ is the heat transfer coefficient. Rutherford et al (1984) obtained the following expression for the heat transfer coefficient $\kappa$ between sinter phonons and $^3$He quasi-particles:

$$\kappa = \kappa_0 \int_0^\infty d \omega \rho(\omega) Yl(Y) \left[ \exp(Y) - 1 \right]^{-1}.$$ 

In this expression $\kappa_0$ is a constant, $\rho(\omega)$ the density of phonon states per grain $Y = \hbar \omega / K_B T$ with $T$ the phonon temperature and $l(Y)$ a dimensionless integral satisfying

$$\lim_{Y \to 0} l(Y) = 2.$$ 

The above result shows that as $T \to 0$, Debye theory yields $\kappa \sim T^3$. In contrast for isolated grains with three translationally invariant modes per grain $\rho(\omega)$ possesses a $\delta$-function at the origin and $\kappa$ tends to a maximum of $6\kappa_0$. This demonstrates that the heat exchange between sinter phonons and $^3$He quasi-particles can be enhanced by decreasing the coupling between the grains. In practice the experimentally measured heat transfer coefficient is formed from a combination of a variety of thermal conductances. As a consequence the optimum sintering conditions will need to be established experimentally.

The problem of describing intermediate-wavelength properties of granular structures is a new topic of theoretical interest. In order to compute such properties we have made use of a new selective renormalisation technique. In this paper, selective renormalisation in $K$-space is used to eliminate irrelevant information from a microscopic model of granularity. In principle this idea can also be developed in a real space by extending the mean-field argument of § 2. Instead of replacing grains by single rigid objects coupled
by renormalised springs, one might attempt to replace a grain by \( r \) rigid objects of volume \( (L/r)^d \), with renormalised inter- and intra-grain couplings. If the couplings are correctly chosen, such a model will describe the dynamical properties of the system at wavelengths \( \lambda > L/r \). This realisation of selective renormalisation remains to be investigated in detail.

It is important to note that theories of granularity may have applications to systems which at first sight appear to be homogeneous. An example is provided by network glasses below their rigidity percolation threshold (Thorpe 1983). In the absence of angular forces, such systems can consist of rigid islands embedded in floppy regions that support no elastic forces. To stabilise the structure, weak angular forces must be included, which form a coupling between the islands. The results of § 4 suggest that such systems will exhibit a low-frequency density-of-states enhancement at wavelengths greater than the size of a typical island. It is interesting that at certain values of the coupling and disorder (e.g. \( \delta = 0.91, 0.45; \sigma^2 = \frac{1}{2}, 1 \) in figure 8) this enhancement manifests itself as a shoulder or broad extremum in \( \rho(\omega) \), which would lead to a crossover from a heat capacity proportional to \( T^3 \) to one proportional to \( T \) at low temperatures \( T \).

In disordered materials these features are attributed to the presence of two-level systems (Anderson et al 1972, Phillips 1972). The results of the present paper demonstrate that in granular structures a linear heat capacity can arise even in the absence of such entities.

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