Excess Vibrational Modes and the Boson Peak in Model Glasses
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The Debye T^3 law is part of the canon of physics: essentially every physics student gets taught in one of the elementary condensed matter physics courses how the low temperature T^3 law of the specific heat of solids in three dimensions simply follows from the ω^{d-1} scaling of the density of states (DOS) of low frequency phonon modes in d dimensions. The scaling of the DOS, of course, simply reflects the phase space of these phonon modes, and this is why the Debye scaling is so ubiquitous and independent of any details.

Clearly, glasses behave as elastic solids at sufficiently long wavelengths and low frequencies, so they exhibit the T^3 Debye scaling at low enough temperatures as well. However, as is well known, glasses exhibit many characteristic deviations from this behavior at intermediate temperatures of order 10 Kelvin — the plateau in the specific heat which has traditionally been interpreted in terms of two-level systems, is a well known example of this. Another more microscopic signature from Raman and neutron scattering is what has been termed the boson peak, a strong anhancement of the DOS of low frequency modes, frequencies corresponding to energies of order tens of Kelvins as well — apparently glasses tend to have an excess of low-frequency vibrational modes. Where does this peak come from? Are these the signatures of two-level systems or is something else happening?

In the paper above, the authors shed new light on this open issue by interpreting it in the light of recent advances in our understanding of granular media. A good model system for granular matter is a collection of particles which interact through repulsive forces which are identically zero beyond some finite range, and which sharply increase as soon as the particles approach each other within this range (this is clearly motivated by the fact that two marbles do not interact till they touch, and strongly repel each other when they are pressed together). The nice aspect of such a model is that contacts are sharply defined — particles interact or they don't. This sharp definition and the possibility to approach the hard sphere limit continuously by increasing the steepness of the potential has allowed researchers to revisit various old problems and shed new light on them. Daan Frenkel reported last month about new advances on the problem of *"random close packing"* of hard spheres. In the present paper, the authors use this line of approach to shed new light on the origin of the boson peak.

A crucial feature of these granular models of compressible particles with finite

range forces is that when the steepness of the potential increases or, equivalently, when the confining pressure is lowered for fixed potential, the packing approaches a *marginal solid*: in that limit, the solid has just enough contacts to allow the forces on each particle to balance. This can be demonstrated quite generally by comparing the number of constraints associated with force balance on each particle and with those associated with the contacts (as in the zero pressure limit two interacting particles have to be separated by precisely the interaction range of the force). At pressures small enough that the particles are only pressed weakly together, one is close to this limit: There are then more contacts than the minimum number necessary to maintain a stable solid, but the excess number of contacts remains small and the DOS is strongly enhanced: there are many low-frequency modes which can be thought of as weakly distorted analogs of the so-called *"floppy modes"* which Alexander introduced for underconstrained systems [1]. Wyart *et al.* [2] have shown that the DOS of such a solid has is *flat* beyond above some lower frequency cutoff ω^* determined by the excess number bonds.

Thus, a natural question to ask is whether the "boson peak", the excess of low frequency vibrational modes that are observed in glasses, is simply the manifestation of the enhancement of the number of low-frequency modes in weakly constrained systems. Of course, in a system like a glass where interactions are longer-ranged and partly attractive, a sharp separation between particles that are in contact and those that are not, is impossible. Nevertheless, from the Weeks-Chandler-Andersen theory of liquids we know that in a dense liquid one can treat the weak and relatively long-ranged attractions as perturbutions about a reference system with harsh repulsive interactions. Very much along the same lines, the authors of this paper show that also in a glass-forming mixture of Lennard-Jones particles there is a well-defined division between a few strong repulsive interactions (stiff contacts) and the more numerous weaker interactions. These weaker interactions include the attractive ones, and can be treated as a correction. Even though these Lennard-Jones glasses have a high coordination number, this separation shows that the effective number of strong contacts that dominates the vibrational properties, is relatively close to the minimum needed for mechanical stability. This is an important step forward in our understanding of the boson peak.

Some of the elements of this approach are reminiscent of the old constraint theory of glasses [3], but the present approach is not limited to co-valently bonded glasses and focusses on the strongly repulsive bonds. It remains to explore these ideas for realistic models for the materials in which the boson peak has been studied experimentally, and to explore possible connections and differences with other anomalies in glassy systems. After all, the phonon energies of the boson peak correspond with thermal energies consistent with the typical temperature range of the plateau in specific heat and thermal conductivity. Thus these are probably two signatures of one and the same effect. However, although the authors do not stress this, the "floppy mode

like" vibrations that cause the enhancement of the DOS typically involve many particles and thus are not very localized, whereas in a two-level system type picture one would expect these modes to be localized on at most a few particles. The picture of the two scenarios thus *is* very different.

References
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