The vibrational dynamics of glasses at the frequencies that control the specific heat in the 1K–100K range is a long-standing physical problem. At the lowest temperatures, an anomalous linear dependence on T can be reproduced by the two-level model \[\hbar\omega_{BP} = \frac{C}{T}\] At slightly higher temperatures, another deviation from the Debye $T^3$ law is found: the specific heat divided by $T^3$ shows a peak near 10K \[\hbar\omega_{BP} = \frac{C}{T}\]. This peak points to the existence of an excess of vibrational states at frequencies $\omega \sim 1 \text{THz}$, which shows as a peak in the plot of $g(\omega)/\omega^2$ ($g(\omega)$ being the vibrational density of states, as obtained by Raman or inelastic neutron scattering). Since the scattering intensity at the peak scales in temperature with Bose statistics, the peak has become known as the Boson Peak (BP). The physical origin of the BP is a matter of a lively debate within the experimental and theoretical glass community.

The recent experimental efforts to elucidate the nature of the high frequency excitations in glasses have produced a wealth of inelastic scattering data (X-ray, Raman and neutrons). These experiments have found a BP on almost all studied glassformers, although of an intensity that varies substantially among different materials. Two of the BP should be remarked. First, the peak can vary substantially among different materials. Two all studied glassformers, although of an intensity that differs among glasses, a wealth of inelastic scattering data (X-ray, Raman and neutrons). These experiments have found a BP on almost all studied glassformers, although of an intensity that varies substantially among different materials. Two features of the BP are available. First, the peak frequency $\omega_{BP}$ is several times smaller than any natural frequency scale, like the Debye frequency or the band edge. Moreover, where good data for the dispersion relation $\omega(p)$ (determined from the the Brillouin peak in the dynamic structure factor, which probes only longitudinal modes) are available, it has been checked that $\omega(p)$ is still a linear function of the momentum p at $\omega_{BP}$. This is the case for glycerol, LiCl:6H$_2$O \[\hbar\omega_{BP} = \frac{C}{T}\], Ca$_{40.4}$K$_{0.6}$ (NO$_3$)$_{1.4}$, B$_2$O$_3$ \[\hbar\omega_{BP} = \frac{C}{T}\], and polybutadiene \[\hbar\omega_{BP} = \frac{C}{T}\]. Silica, however, shows the opposite behavior \[\hbar\omega_{BP} = \frac{C}{T}\]. Yet, in silica the BP evolution upon increasing the density has been studied experimentally \[\hbar\omega_{BP} = \frac{C}{T}\] and in simulations \[\hbar\omega_{BP} = \frac{C}{T}\]. In close agreement with the results presented here, it was found that $\omega_{BP}$ shifts to larger frequencies and the BP looses intensity when the density grows. The BP has also been identified in the dynamic structure factor at high exchanged momentum, both experimentally \[\hbar\omega_{BP} = \frac{C}{T}\] and in simulations \[\hbar\omega_{BP} = \frac{C}{T}\], which reflects the fact that the dynamic structure factor tends to fail within the experimental and theoretical glass community.

Perhaps the only widely-agreed upon statement about the BP is that, as well as the whole dynamic structure factor in this frequency region, can be understood invoking only harmonic vibrations \[\hbar\omega_{BP} = \frac{C}{T}\]. Yet, in silica the BP evolution upon increasing the density has been studied experimentally \[\hbar\omega_{BP} = \frac{C}{T}\] and in simulations \[\hbar\omega_{BP} = \frac{C}{T}\]. In close agreement with the results presented here, it was found that $\omega_{BP}$ shifts to larger frequencies and the BP looses intensity when the density grows. The BP has also been identified in the dynamic structure factor at high exchanged momentum, both experimentally \[\hbar\omega_{BP} = \frac{C}{T}\] and in simulations \[\hbar\omega_{BP} = \frac{C}{T}\], which reflects the fact that the dynamic structure factor tends to fail within the experimental and theoretical glass community.

In this Letter we discuss analytically and numerically an off-lattice model of scalar harmonic vibrations, which is a problem on random-matrix theory \[\hbar\omega_{BP} = \frac{C}{T}\], showing that it has a Boson peak with the above-mentioned experimentally identified characteristics. Thus it is unnecessary to invoke anharmonicity or transverse modes to explain the BP (although they are certainly present in...
real glasses), which instead, as we will show, arises from the hybridization of extended but non-propagating modes with sound waves, induced by a mechanical instability. Our model consists in particles oscillating harmonically around (disordered) equilibrium positions, along a fixed direction \( \mathbf{u} \) (i.e. we neglect all transverse modes): \( \mathbf{x}_i(t) = \mathbf{x}_i^{eq} + \mathbf{u} \phi_i(t), 1, \ldots, N \). The potential energy is \( V = \frac{1}{2} \sum_{i,j} f(\mathbf{x}_i^{eq} - \mathbf{x}_j^{eq}) (\phi_i - \phi_j)^2 = \sum_{i,j} \phi_i M_{ij} \phi_j \), where \( f \) is the second derivative of the pair potential and the dynamical matrix matrix (Hessian) is

\[
M_{ij} = \delta_{ij} \sum_{k=1}^N f(\mathbf{x}_i^{eq} - \mathbf{x}_k^{eq}) - f(\mathbf{x}_i^{eq} - \mathbf{x}_j^{eq}).
\]

The model is completely defined when \( f \) and the distribution of the \( \mathbf{x}^{eq} \) are chosen. We take the latter uniform in the whole volume, while \( f \) is taken to be regular at short distances. As discussed in Ref. \( \text{[10]} \), this is a good first approximation to the correlations of the \( \mathbf{x}^{eq} \). We shall consider the family of functions

\[
f_\alpha(r) = (1 - \alpha r^2/\sigma^2) e^{-r^2/(2\sigma^2)},
\]

where \( 0 < \alpha < 0.2 \) (the upper bound has to be imposed in order to guarantee a positive sound velocity). When \( \alpha = 0 \) (Gaussian case), the hessian is strictly positive. When \( \alpha > 0 \), we have a stable elastic solid at high particle-number density, \( \rho \), while at low enough \( \rho \), typical interparticle distances will be large enough to allow negative eigenvalues (imaginary frequencies). Therefore the density controls the appearance of a mechanical instability in this model: there is a phase-transition from the density controls the appearance of a mechanical instability (i.e. on lowering the density). As \( \rho \) is reduced, the peak grows (relative to the Debye value, also plotted) and moves to lower \( \omega \). The peak lies always in the linear region of the dispersion relation (Fig. 1, bottom). Since decreasing \( \rho \) plays the role of increasing temperature in our model, the experimental features of the BP are reproduced, without transverse or optical modes or anharmonicity, as claimed.

Let us discuss analytically the BP found in our model. Within our random-matrix approach \( \text{[16, 31]} \), the DOS is obtained from the resolvent \( G(p, z) = (1/N) \sum_{jk} \text{exp} \{i \mathbf{p} \cdot (\mathbf{x}_i^{eq} - \mathbf{x}_k^{eq}) \} [(z - M)^{-1}]_{jk} \), where the overline stands for the average over \( \mathbf{x}^{eq} \). Defining \( G(z) = G(p = \infty, z) \), the DOS is \( g(\omega) = -\frac{\pi}{\rho} \text{Im} G(\omega^2 + i0^+) \). Expanding the resolvent in \( 1/\rho \) \( \text{[16]} \) and resumming an infinite subset of diagrams \( \text{[17]} \), a non-linear equation is found for \( G(p, z) \) that in the \( p \to \infty \) limit yields

\[
\frac{1}{\rho G(z)} = \frac{z}{\rho} - \hat{f}(0) - AG(z) - \int \frac{d^3 q}{(2\pi)^3} \hat{f}^2(q) G(q, z),
\]

where \( A = (2\pi)^{-3} \int \hat{f}^2(q) \, d^3 q \) and \( \hat{f}(q) \) is the Fourier transform of \( f(r) \). With this equation, one needs to know the resolvent at all \( q \) to obtain the DOS, due to the last term in the r.h.s. This can be done by solving numerically the self-consistent equation of ref. \( \text{[17]} \). Here we perform an approximate analysis, which is more illuminating. The crudest approximation is to neglect this term, in which case Eq. \( \text{3} \) is quadratic in \( G \), and one easily finds a semicircular DOS, with center at \( \omega_c = \rho \hat{f}(0) \) and radius \( 2\sqrt{\rho A} \).

Indeed, when \( \rho \to \infty \), the spectrum is made of plane waves, with dispersion relation \( \omega^2(p) = \rho (\hat{f}(0) - \hat{f}(p)) \). \( \text{[16, 31]} \) (a continuous elastic medium). \( \omega(p) \) in \( g(\omega)/\omega^2 \) arises on approaching the instability (i.e. on lowering the density). As \( \rho \) is reduced, the peak grows (relative to the Debye value, also plotted) and moves to lower \( \omega \). The peak lies always in the linear region of the dispersion relation (Fig. 1, bottom). Since decreasing \( \rho \) plays the role of increasing temperature in our model, the experimental features of the BP are reproduced, without transverse or optical modes or anharmonicity, as claimed.
saturates for large $p$ at $\omega^2 = \rho \hat{f}(0)$, yielding an enormous pile-up of extended (but non-propagating) states which causes the DOS to be concentrated at this frequency $\omega^*$. This is the glass analogue of a van-Hove singularity. At finite $\rho$, the density fluctuations of the $z$-axis split this degeneracy, and yield the semicircular part of the spectrum at high frequency that can be recognized in the upper panel of Fig. 1. But the semicircular spectrum misses the Debye part, and a better approximation is needed. So we substitute $G$ in the last term of the r.h.s. by the resolvent of the continuum elastic medium

$$G_0(z, p) = (z - \omega^2(p))^{-1}.$$ This is reasonable because the $f^2(q)$ factor makes low momenta dominate the integral, and due to translational invariance $G(z, p) \approx G_0(z, p)$ in this region $[16]$. We shall be looking at small $\omega$, so to a good approximation

$$\int \frac{d^3q}{(2\pi)^3} \hat{f}^2(q)G_0(q, z) \approx -\frac{1}{\rho} B - i\frac{\rho\hat{f}^2(0)}{4\pi c^3} \omega, \quad (4)$$

where the sound velocity is $c = \sqrt{\rho \hat{f}''(0)/2}$, while $B$ is a positive constant. Then Eq. (3) is again quadratic in $G$, and can be solved to give

$$G(\omega^2 + i0^+) \approx \frac{\omega^2 - \rho \hat{f}(0) + i\rho\hat{f}^2(0)\omega}{2\rho A} \times \left(1 - \frac{4\rho A}{\omega^2 - \rho \hat{f}(0) + i\rho\hat{f}^2(0)}\right). \quad (5)$$

We have two limiting cases. At high densities and low frequencies ($\rho \hat{f}(0) \gg \omega^2, B, 2\sqrt{\rho A}$, i.e. when the semicircular part of the DOS does not reach low frequencies, the square root can be Taylor-expanded, and one gets

$$g(\omega) \approx \frac{\omega^2}{2\pi\rho c^3}, \quad (6)$$

which is precisely Debye’s law. At small densities, on the other hand, the center of the semicircle (which is at $\omega^2 = \rho \hat{f}(0) - B$) starts to be comparable to its radius ($\propto \sqrt{\rho}$), implying that the states in the semicircle hybridize with the sound waves. This is the source of the mechanical instability we find numerically in Fig. 1. Mathematically, the instability arises when $G(0)$ develops an imaginary part. This can only come from the square root in Eq. (3), and it will happen for $\rho < \rho_c$, with $\rho_c$ fixed by the condition $2\sqrt{\rho A} + B = \rho_c \hat{f}(0).$ Now when $\rho \gg \rho_c$ and $\omega \ll \omega^* = 2\pi c^3\sqrt{\rho_c A}/(\rho_c \hat{f}^2(0))$, the square root in Eq. (3) behaves as

$$\sqrt{D(\rho - \rho_c) - i\omega/\omega^*}, \quad (7)$$

with $D$ a positive constant. One distinguishes two regimes:

- $\omega^* D(\rho - \rho_c) \ll \omega \ll \omega^*$: the imaginary part of $G$ is proportional to $\sqrt{\omega}$, the DOS being $g(\omega) \propto \omega^{3/2}$.

One thus identify $\omega_{BP}$ with $\omega^* D(\rho - \rho_c)$ that, on approaching the instability, becomes arbitrarily small compared to any natural frequency scale. The mechanical instability is a phase transition, for which the order parameter is $-\text{Im} G(0)$. From Eq. (7) we see that this order parameter behaves as $(\rho_c - \rho)^\beta$, with $\beta = 1/2$, like in mean-field theories. In this sense, we can say that Eq. (3) is a mean-field theory for the model. That our qualitative analysis is correct can be checked looking at Fig. 2, where we show the DOS, and the behavior of $-\text{Im} G(0)$ with $\rho$, both obtained from the self-consistent $G(q, z)$. Note also that the analytical solution compares reasonably well with the numerical solution (Fig. 1) on a qualitative level (though it overestimates $\rho_c$, and likely finds the wrong critical exponent). Since the behavior of the propagator at high momentum does not strongly affect the dispersion relation $[17]$, we do not expect deviations from a linear dispersion relation at $\omega_{BP}$. This can be checked either numerically (Fig. 1, bottom) or solving numerically the self-consistency equations. This is in sharp contrast with lattice models for the BP $[24, 25]$.

Indeed, on the lattice the DOS is given by the integral of the dynamic structure factor, which is dominated by the Brillouin-peak. Thus the so-called lattice BP reflects a non smooth behavior of the Brillouin-peak. In fact, one can check (Fig. 3) that in these models the BP arise from a transverse van-Hove singularity that affects strongly the longitudinal dispersion relation.

In summary, we have discussed an harmonic model for...
the high frequency dynamics of glasses, without transverse modes. The model has a mechanical instability transition controlled by the density. We have studied the model numerically, and analytically with a mean-field theory for the instability transition. The vibrational spectrum contains a BP which is the precursor of the transition. The BP in our model shares the main features of the experimental BP: it appears for frequencies in the linear part of the dispersion relation and it shifts towards arbitrarily low frequencies on approaching a mechanical instability. We also reproduces qualitatively the behaviour of the silica BP when the density changes [12,13] (the detailed theory of the temperature evolution of the silica BP should consider its negative thermal dilatation coefficient). The BP is built from the hybridization of sound waves with high frequency modes (extended but non-propagating) that get softer upon approaching the instability. The analogues of our instability transition in nature is the topological phase transition [33] that underlies the dynamic crossover at the Mode Coupling temperature of real glasses [22]. The precise nature of the high-frequency modes that hybridize with the sound-waves is most likely material dependent and non-universal: they could be transverse [4,15,20,26], optical [13], or even longitudinal modes as in our model. We believe however that the basic mechanism for the formation of the BP uncovered in our model is common to most (if not all) the structural glasses. Yet all real glasses do have transverse excitations, and one could ask about generic new features introduced by these modes. We are currently working to extend the present theory in this direction.

We thank G. Ruocco, O. Pilla and G. Viliani for discussions. TSG was supported in part by CONICET (Argentina), and VMM by E.C. contract HPMF-CT-2000-00450.

[1] P. W. Anderson et al., Philos. Mag. 25, 1 (1972); W. A. Philips, J. Low. Temp. Phys. 7, 351 (1972).
[2] R. O. Pohl, in Amorphous solids — Low temperature properties, Topics in current physics 24, edited by W. A. Philips, Springer, Berlin (1981).
[3] C. Masciovecchio et al., Phys. Rev. Lett. 76, 3356 (1996); F. Sette et al., Science 280, 1550 (1998).
[4] A. Matic et al., Europhys. Lett. 54, 77 (2001).
[5] C. Masciovecchio et al., Phys. Rev. B 55, 8049 (1997); P. Benassi et al., Phys. Rev. Lett. 77, 3835 (1996).
[6] D. Fioretto et al., Phys. Rev. E 59, 1470 (1999).
[7] O. Pilla et al, Phys. Rev. Lett. 85, 2136 (2000); M. Foret et al., Phys. Rev. Lett. 78, 4669 (1997).
[8] A. P. Sokolov et al., Phys. Rev. B 52, R9815 (1995).
[9] N. J. Tao et al., Phys. Rev. A 44, 6665 (1991).
[10] D. Engberg et al., Phys. Rev. B 59, 4053 (1999).
[11] A. Wischnewski et al., Phys. Rev. B 57, 2636 (1998).
[12] S. Sugai and A. Onodera, Phys. Rev. Lett. 77; Y. Inamura et al., Physica B 241-243, 903 (1998); Y. Inamura et al., Physica B 263-264, 299 (1999).
[13] P. Junod and R. Jullien, J. Chem. Phys. 113, 2768 (2000); O. Pilla, private communication.
[14] B. Hehlen et al., talk at the APS March meeting 2001, Seattle; E. Courtens, talk at the International Discussion Meeting on Slow Relaxations 2001, Creta; L. Brjeson et al., talk at the APS March meeting 2001, Seattle.
[15] J. Horbach et al., Eur. Phys. J. B 19, 531 (2001).
[16] V. Martin-Mayor et al. J. Chem. Phys. 114, 8068 (2001); T. S. Grigera et al., cond-mat/0104433.
[17] T. S. Grigera et al., Phys. Rev. Lett. 87 085502 (2001).
[18] J. Horbach et al. J. Phys. Chem. B 103, 4104 (1999).
[19] S. N. Taraskin and S. R. Elliot, Phys. Rev. B 59, 8572 (1999).
[20] G. Ruocco et al., Phys. Rev. Lett. 84, 5788 (2000).
[21] W. Götze and M. R. Mayer, Phys. Rev. E 61, 587 (2000).
[22] W. Schirmacher et al., Phys. Rev. Lett. 81, 136 (1998).
[23] S. N. Taraskin et al., Phys. Rev. Lett. 86, 1255 (2001); Simdyankin et al., cond-mat/0108336.
[24] J. W. Kantelhardt et al., Phys. Rev. B 63, 064302 (2001).
[25] V. G. Karpo zov et al., Sov. Phys. JETP 57, 439 (1983); U. Buchenau et al., Phys. Rev. B 46, 2798 (1992).
[26] M. Sampoli et al., Phys. Rev. Lett. 79, 1678 (1997).
[27] M. Foret et al., Phys. Rev. Lett. 77, 3831 (1996).
[28] D. A. Parshin and C. Laermans, Phys. Rev. B 59, 132203 (2001).
[29] M. L. Metha, Random matrices, Academic Press (1991).
[30] T. Thee haus et al., cond-mat/0105391.
[31] M. Mézard et al., Nucl. Phys. B559, 689 (1999).
[32] W. Götze and L. Sigogren, , Rep. Prog. Prog. Phys. 55 241 (1992); W. Kob and H. C. Andersen, Phys. Rev. Lett. 73, 1376 (1994).
[33] L. Angelani et al., Phys. Rev. Lett. 85 5356 (2001); K. Broderix at al., Phys. Rev. Lett. 85 5360 (2001).
[34] C. Benoit et al., J. Phys.: Condens. Matter 4, 3125 (1992) and references therein; P. Turchi et al., J. Phys. C 15, 2891 (1982).