Quasi-localized Vibrations, Boson Peak and Tunneling in Glasses

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The most basic property of glasses and amorphous materials is their structural disorder. The amorphous structures are strongly restricted by the strong repulsive forces on nearest neighbour distances or nearest neighbour bonds, both effecting local order. The disorder causes local strains which destabilize the glass locally. This local softness is apparent in the quasi-localized vibrations (QLV). These are soft localized vibrations hybridized with the sound wave phonons. The resulting exact harmonic eigenstates resemble sound waves with “random noise”. To avoid stressing the strong nearest bonds the cores of the QLV extend over ten or more atoms or molecules. The atomic structures of the QLV reflects the local geometry of the glass. In SiO_2 one finds twisting of tetrahedra, in metals chains of atoms move simultaneously. QLV have been directly observed in numerous simulations. Amongst others they have been used to explain diffusion and the time dependence of the dynamic heterogeneity [1].

We show that both the vibrational Boson peak (BP) and the two level systems (TLS) in glasses are directly linked to these quasi-localized vibrations [2]. Extending the soft potential model we show that a distribution of soft localized modes interacting with sound waves leads to both the BP in vibration and the TLS. The interaction between the localized modes and the sound waves induces a dipole interaction between the localized modes causing a shift of their
eigenvalues, some of them becoming negative, in harmonic approximation the system is unstable. The low frequency eigenvalue spectrum resembles the one for weakly unstable random matrices. In this description the dynamic matrix is written in mode-space. Converted to real space this implies a correlation of the force constant disorder. Anharmonicity stabilizes the system in a nearby minimum. The new harmonic excess vibrational spectrum has, independent of the actual strength of the anharmonicity, a universal shape in agreement with the measured BP. This mechanism also explains the shift of the BP under applied pressure. The same process forms, out of some of the previously unstable harmonic modes, TLS's. The theory predicts in a natural way the observed small density of TLS's.

References

[1] -F. Faupel *et al.*, Rev. Mod. Phys. **75,** 237 (2003).
[2] -D. A. Parshin, H. R. Schober and V. L. Gurevich, Phys. Rev. B **76,** 064206 (2007) .