GLASS TRANSITIONS

Quantum glass forging

Intuition suggests that the occurrence of large quantum fluctuations should prevent a material from forming a glass, yet theory and simulations that explicitly incorporate such fluctuations suggest the opposite could be true.

Francesco Zamponi

There has been spectacular progress over the past three decades in the development of a theory of classical glasses. Pioneering studies of correlations between the dynamic parameters that describe glass-forming materials has revealed that the glass transition is the result of a collective phenomenon. Close to the transition, the number of microscopic elements (atoms, molecules) that need to move together to relax any local perturbation increases sharply. This rapidly leads to a dynamical arrest that freezes these elements into a solid structure. Such long-range correlations produce universal behaviour across a diverse variety of systems, including silica glasses, emulsions, polymers and granular materials. Although most examples of glass forming are classical and occur at temperatures well above those at which quantum effects become important, there are notable exceptions. Yet, despite the aforementioned success in modelling wholly classical glass transitions, little progress has been made towards extending them to include the influence of quantum fluctuations. Writing in *Nature Physics*[1], Markland and colleagues describe a theory that addresses this shortcoming.

Most descriptions of phase transitions use mean-field theory as their starting point. This describes the interaction potential of a single atom in terms of a 'mean field' determined self-consistently from the average of its interaction with all other atoms in the system. This turns a complex many-body problem into a more computationally tractable single-body problem. Mean-field theory predicts that the glass transition is driven by an underlying phase transition at which an 'entropy crisis' occurs — a point at which the entropy associated with the number of distinct local structures a liquid can form falls to zero. This is a strange kind of phase transition — called a random first-order transition (RFOT) — which is a second-order thermodynamic transition, but shares several important aspects of first-order transitions, such as metastability and the role of nucleation[2,3].

The dynamic part of RFOT theory is called mode-coupling theory (MCT)[4], and was developed in the context of critical phenomena. The thermodynamic part of RFOT theory is called replica theory, and was developed as a general tool for studying disordered systems[5]. As for any mean-field theory, the validity of RFOT theory should be discussed with extreme care. It is well known in the context of critical phenomena that fluctuations around the mean-field approximation can dramatically affect the behaviour of a system, and in some cases completely wash out the transition. However, even in situations where mean-field predictions are heavily altered by fluctuations, mean-field theory can retain its quantitative validity for systems far enough from their critical point and whose correlations are only moderately long-ranged. Moreover, both MCT and replica theory agree well with experiments and numerical simulations[4,5].

Several authors attempted to build a theory of quantum glasses[6,7], but none has so far been able to obtain quantitative results for realistic systems. That is, until now with the quantum glass picture developed by Markland *et al.*[1], which they have applied to an ensemble of quantum hard spheres, with surprising results. Basic intuition suggests that increasing the strength of quantum fluctuations should enable atoms to better explore the phase space through tunnelling, and thereby inhibit the onset of dynamical arrest that is necessary for glass formation. In contrast, Markland *et al.* find that increasing quantum fluctuations in a system by increasing the thermal wavelength of its particles (by reducing their mass) actually decreases the packing fraction at which it forms a glass. Path integral numerical simulations performed by the authors corroborate this behaviour and provide an explanation: quantum fluctuations increase the effective radius of the particles, thereby increasing the effective packing density, slowing down the dynamics and promoting arrest.

There are many potential systems beyond the simple system Markland *et al.* study to which their quantum glass

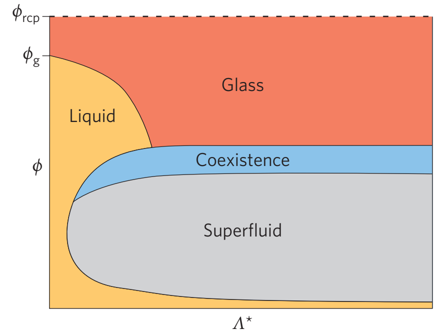

Figure 1 | Possible phase diagram of quantum hard spheres in the presence of bosonic exchange, adapted from refs 1 and 10. ϕ is the fraction of volume occupied by the spheres, and Λ^* is the De Broglie thermal wavelength of the particles, ϕ_g is the packing fraction for a classical glass transition and ϕ_{rcp} is the random close-packing density. The liquid–glass transition line has been determined by Markland *et al.*, but they could not investigate the superfluid transition because exchange was neglected. The superfluid transition can be first or second order; in the first-order case the transition is accompanied by phase coexistence. Note that at very low temperature Λ^* is large, therefore there is always a first-order transition between the superfluid and a non-superfluid glass.

model could be applied. Perhaps the most intriguing is that of disordered solid helium-4, which recent experiments suggest could form a supersolid phase[8] — an exotic quantum phase that simultaneously exhibits characteristics both of a solid and a superfluid[9]. Could such phenomena arise in a quantum glass? To answer this requires a model that includes bosonic statistics, which is absent in the theory of Markland *et al.* Evidence for similar re-entrant behaviour to those presented by Markland *et al.* has recently been reported in static calculations based on a lattice model[10], confirming that RFOT models can produce consistent dynamic and thermodynamic predictions. Such calculations lend themselves more easily to including bosonic exchange, and suggest that it can indeed result in a first-order superfluid to (non-superfluid) glass phase transition. This transition is accompanied by a region of coexistence of the two phases (Fig. 1). Is this result an artefact of the lattice? Or could it explain at least some of the experiments on disordered solid helium? Is it possible to make more quantitative calculations on a realistic model of helium, in the presence of exchange?

Another potential application is the study of a class of models that are used to describe the dynamics of computer algorithms built to solve computationally difficult problems. The danger of such algorithms failing to find an optimal solution to a problem by becoming trapped in local minima is well known, and directly analogous to the dynamical arrest that induces a glass transition. It has been conjectured that quantum computers might overcome this[11]. Whether they will behave the way we expect them to, particularly in light of the counter-intuitive phenomena observed in the present work, is an open question. But at least if they do throw up any surprises, models like those developed by Markland *et al.* should help us better understand, and hopefully overcome, these problems too. ❐

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NONLINEAR DYNAMICS

Quantum pendula locked in

A study of the autoresonant behaviour of a superconducting pendulum reveals that quantum fluctuations determine only the initial oscillator motion and not its subsequent dynamics. This could be important in the development of more efficient methods for reading solid-state qubits.

Adrian Lupascu

The frequency of a nonlinear oscillator can become synchronized with a chirped driving force of decreasing frequency, which results in efficient energy transfer. Such behaviour — known as autoresonance — only occurs when the amplitude of the driving force exceeds a certain threshold. The value of this threshold is determined by the initial state of the oscillator, which in turn is influenced by fluctuations in the system induced by its environment. As they report in *Nature Physics*[1], Murch and colleagues extend the study of autoresonance to the quantum regime. The interplay of nonlinearities and quantum fluctuations is intriguing. As expected, quantum fluctuations have a role in the system dynamics. However, the way in which these fluctuations come into play is surprising: they make the initial state 'uncertain', but play no role in subsequent system dynamics. Understanding the role of quantum fluctuations is essential for sensors based on autoresonance.

Resonance is one of the most familiar concepts in physics. Classically, it is described in terms of the response of a harmonic oscillator to a harmonic driving force. It is usually discussed in the context of a simple linear oscillator, with potential $V(x) = kx^2/2$, where k is the oscillator spring constant and x is its displacement from the mean. This provides a remarkably accurate description of the dynamics of many different systems, including mechanical oscillators, resonant electrical circuits, phonon modes in solids, Fabry–Perot resonators and molecular vibrations. This makes life easier for theoreticians, and is a consequence of the fact that most degrees of freedom of many systems are only weakly excited at moderate driving amplitudes. Nonetheless, there are many systems, particularly in the field of electronics, for which this isn't the case. And they exhibit much richer phenomena. Indeed, the mathematician Stanislaw Ulam once suggested that using the term 'nonlinear systems' is equivalent to describing the bulk of zoology as "the study of non-elephants"[2].

The archetypal nonlinear system is the Duffing oscillator, which can be thought of as a mechanical oscillator, such as a mass connected to a spring, but one whose spring 'constant' is not constant at all; instead, it is dependent on position, so that $k(x) = k_0 - \gamma x^2$, where γ is a constant. The addition of the nonlinear term, γx^2, has important consequences. It causes the resonant frequency of the oscillator to be amplitude-dependent. And for a driving frequency below the small-oscillation natural frequency and large enough amplitude, two oscillation states are possible: a low-amplitude state (where the oscillator sees the excitation as non-resonant) or a high-amplitude state (where the resonant frequency is reduced and therefore driving is more effective). Crucially, the driving parameters (that is, mass and/or spring constant) that induce the system to switch from one state to the other are sensitively dependent on the initial conditions of the oscillator. This effect has the potential to increase mass detection sensitivity[3], and it has been used to detect the state of superconducting quantum two-level systems or quantum bits (see ref. 4 and references therein).

Another intriguing and potentially useful characteristic of nonlinear oscillators is their ability to undergo autoresonant behaviour. For a linear oscillator, the optimum transfer of energy from a driving force occurs at exactly the resonant frequency, which in the ideal case is constant regardless of the amplitude of the oscillation. But for a nonlinear oscillation, as has already been noted, the resonant frequency changes as its amplitude increases, so the frequency of the driving force must