thesis

Quantum crystals

For more than 150 years, physicists have recognized the temperature of matter as reflecting the disorganized energy that it holds. In a simple gas, higher temperature translates into higher average velocities of atoms or molecules in random motion. When particles interact through chemical forces, as in solids and liquids, the forces at work complicate the story, and temperature reflects, more abstractly, the typical disorganized energy in any degree of freedom, or possible dynamical mode, of the system. Often, this energy falls equally across all such modes.

It needn't do so, as Enrico Fermi, John Pasta, and Stanislaw Ulam first showed in 1953; in some nonlinear systems, energy can get trapped in coherent and persisting collective patterns. There are other exceptions too. Cool a simple solid down to very low temperatures, and one might expect the typical kinetic energy of any particle to fall in proportion to *T*, gradually approaching zero. Yet, for solids made of the simplest elements — say, hydrogen or helium — this just isn't true. For helium, experiments find that the kinetic energy of a typical atom at ultracold temperatures, and relatively high pressure, approaches a finite value around 24 K — higher than *T* by many orders of magnitude. The thermodynamic intuition is spectacularly wrong.

Of course, this errant intuition is also about one century out of date. What stands in its way is quantum theory, and limits on fluctuations of dynamical variables as described by the uncertainty principle, which imply that there cannot be a complete quiescence of the particles at zero temperature. Quantum restrictions also account for this strange amplification of kinetic energy. But the story is subtle, for not all solids behave this way. This class of so-called quantum crystals has unique properties, and presents a fascinating challenge for modern physics (C. Cazorla and J. Boronat, *Rev. Mod. Phys.* **89**, 035003; 2017).

As is often the case, the value of an appropriate dimensionless parameter identifies distinct regions of crystal behaviour: classical versus quantum. This parameter known as the de Boer parameter — is the ratio of the typical de Broglie wavelength associated with particles to the distance between them, as determined by interatomic forces. This turns out to depend inversely on the square root of the product of the atomic mass and interaction strength. When



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the de Boer parameter is small, classical behaviour obtains; when it is roughly one or larger, then quantum aspects of the physics instead play a dominant role.

Hence, we should expect solids of heavy and strongly interacting particles anything from salts to diamond or most metallic crystals — to display largely classical structural properties, like those described in textbooks, with atoms vibrating gently around the positions that minimize their potential energy. Each atom or molecule carries kinetic energy of order kT, where k is Boltzmann's constant, and this energy decreases regularly as temperature falls to zero. In contrast, materials with much lighter particles and weaker interactions deviate strongly into quantum territory. Modern experiments reveal their profoundly different structures and dynamic behaviour.

Bulk molecular hydrogen solidifies at sufficiently low temperature - below around 14 K — and will do so even under conditions of zero pressure. How tightly molecules rest in their equilibrium positions is reflected in the so-called Lindemann ratio of the mean squared displacement to the basic lattice distance, which for hydrogen is around 0.1. This isn't as impressive as helium; both isotopes (4He and 3He) solidify at sufficiently low temperatures under moderate pressures. with a Lindemann ratio of about 0.3. This implies that it is not unusual for atoms to move nearly half the distance towards neighbouring atoms. These large excursions also lead to a strongly nonlinear character of atomic motions, as atoms explore regions of the interatomic potential well outside of the linear harmonic region.

More strikingly, the quantum crystalline nature in helium reveals itself in another way. The resulting atomic fluctuations are strong enough to completely prevent the solidification of the system, even at T = 0, under conditions of zero pressure. This is quite unlike hydrogen. The phase transition in the solid state that would be a foregone conclusion, classically, does not take place.

These phenomena are now all well understood, and Cazorla and Boronat review the many modern theoretical and experimental techniques developed to study them, not only in solids of pure elements such as lithium or compounds such as methane or lithium hydride, but also in more exotic substances such as Wigner crystals in electron gases, and vortex lattices in superconductors. But other aspects of quantum crystals remain much more mysterious. In these highly dynamic solids, for example, crystalline defects do some surprising things.

The shear modulus of a solid measures its stiffness in response to an applied shear stress. In ⁴He, experiments indicate that the shear modulus, μ , increases with decreasing temperature below about 0.15 K, and this seems linked to the behaviour of defects. In particular, line defects at these lower temperatures seem to get pinned to ³He impurities, despite these representing only 200 parts per billion of ⁴He atoms. Above 0.15 K, the defects become mobile, and the crystal becomes easier to deform. The transition marks a boundary at which helium begins to exhibit supersolidity — the analogue of superfluidity in a quantum solid.

Another finding goes in the opposite direction — towards an apparent complete lack of stiffness. Experiments with ultrapure single crystals of ⁴He indicate that at a temperature of around 0.1 K, the resistance to shear applied along one particular direction suddenly vanishes, while the elastic behaviour in other directions remains completely normal. This weird and unexpected effect has been called giant plasticity, and its potential cause remains a topic for debate. Theorists suspect that dislocations and isotopic impurities are likely interacting in peculiar ways - dislocations may, for example, take on quantum aspects themselves and delocalize across the lattice but are far from understanding how.

Quantum solids may have been created on Earth nearly a century ago, but they could have existed elsewhere in the Universe long before. In their review, Cazorla and Boronat give a glimpse of the many surprises these systems keep turning out, in things like thin films, small clusters of atoms and materials such as ferroelectrics. When quantum effects are important, much of what we once thought we knew about simple solids just isn't so.

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