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This article may be too technical for most readers to understand. Please help improve it to make it understandable to non-experts, without removing the technical details. (July 2022) (Learn how and when to remove this template message) Statistical mechanics Thermodynamics Kinetic theory Particle statistics Spin-statistics theorem Identical particles Maxwell-Boltzmann Bose-Einstein Fermi-Dirac Parastatistics Anyonic statistics Braids statistics Thermodynamic ensembles NVE Microcanonical μ VT Grand canonical NPH Isoenthalpic-isobaric NPT Isothermal-isobaric Models Debye Einstein Ising Potts Potentials Internal energy Enthalpy Helmholtz free energy Gibbs free energy Grand potential / Landau free energy Scientists Maxwell Boltzmann Gibbs Einstein Ehrenfest von Neumann Tolman Debye Fermi Bose etc The Einstein solid is a model of a crystalline solid that contains a large number of independent three-dimensional quantum harmonic oscillators of the same frequency. The independence assumption is relaxed in the Debye model. While the model provides qualitative agreement with experimental data, especially for the high-temperature limit, these oscillations are in fact phonons, or collective modes involving many atoms. Albert Einstein was aware that getting the frequency of the actual oscillations would be difficult, but he nevertheless proposed this theory because it was a particularly clear demonstration that quantum mechanics could solve the specific heat problem in classical mechanics.[1] Historical impact The original theory proposed by Einstein in 1907 has great historical relevance. The heat capacity of solids as predicted by the empirical Dulong-Petit law was required by classical mechanics, the specific heat of solids should be independent of temperature. But experiments at low temperatures showed that the heat capacity changes, going to zero at absolute zero. As the temperature goes up, the specific heat goes up until it approaches the Dulong and Petit prediction at high temperature. By employing Planck's mechanics. Heat capacity For a thermodynamic approach, the heat capacity can be derived using different statistical ensembles. All solutions are equivalent at the thermodynamic limit. Microcanonical ensemble Heat capacity of an Einstein solid as a function of temperature. Experimental value of $3Nk$ is recovered at high temperatures. The heat capacity of an object at constant volume V is defined through the internal energy U as $C_V = (\partial U / \partial T)_V$. The temperature of the system, can be found from the entropy $I_T = S / k$. To find the entropy consider a solid made of N atoms, each of which has 3 degrees of freedom. So there are $3N$ quantum harmonic oscillators (hereafter SHOs for "Simple Harmonic Oscillators"). $N = 3N$ Possible energies of an SHO are given by $E_n = \hbar\omega(n + 1/2)$, or, in other words, the energy levels are evenly spaced and one can define a quantum of energy $\epsilon = \hbar\omega$ which the energy of an SHO is increased. Next, we must compute the multiplicity of the system. That is, compute the number of ways to distribute q quanta of energy among N boxes or separating stacks of pebbles with $N - 1$ partitions or arranging q pebbles and $N - 1$ partitions. The last picture is the most telling. The number of arrangements of n objects is $n!$. So the number of possible distinguishable arrangements one has to divide the total number of arrangements by the number of indistinguishable arrangements. There are $q!$ identical partition arrangements, and $(N - 1)!$ identical partition arrangements. Therefore, multiplicity of the system is given by $\Omega = (q + N - 1)! / (q! (N - 1)!)$. With the help of Stirling's approximation, entropy can be simplified: $S / k = \ln(\Omega) \approx \ln(N^q) + q\ln(q) - q\ln(N + q)$. Since there are q energy quanta total in the system in addition to the ground state energy of each oscillator. Some authors, such as Schroeder, omit this ground state energy in their definition of the total energy of an Einstein solid. We are now ready to compute the temperature $T = \partial S / \partial U = \partial S / \partial q dU = k \ln((1 + N^q) / q)$. The first term is associated with zero point energy and does not contribute to specific heat. It will therefore be lost in the next step. Differentiating with respect to temperature to find $C_V = \partial U / \partial T$, we obtain: $C_V = \varepsilon / k T = N^2 e^2 k T^2 e^2 / k T = e^2 / k T - 1$. Although the Einstein model of the solid predicts the heat capacity accurately at high temperatures, and in this limit $T \rightarrow \infty$, $C_V = 3Nk$, which is equivalent to Dulong-Petit law. Nevertheless, the heat capacity noticeably deviates from experimental values at low temperatures. See Debye model for how to calculate accurate low-temperature heat capacities. Canonical ensemble Heat capacity is obtained through the use of the canonical partition function of a simple quantum harmonic oscillator. $Z = \sum_n e^{-\epsilon_n / kT}$ where $\epsilon_n = (n + 1/2)\hbar\omega$. The partition function formula yields $Z = \sum_n e^{-\epsilon_n / kT} = e^{-\epsilon_1 / kT} + e^{-\epsilon_2 / kT} + \dots + e^{-\epsilon_N / kT}$. Substituting this into the partition function formula yields $Z = \sum_{n=0}^{\infty} e^{-\epsilon_{n+1/2} / kT} = e^{-\epsilon_{1/2} / kT} + e^{-\epsilon_{3/2} / kT} + \dots + e^{-\epsilon_{N+1/2} / kT}$. This is the partition function of one harmonic oscillator. Because, statistically, heat capacity, energy, and entropy of the solid are equally distributed among its atoms, we can work with this partition function to obtain those quantities and then simply multiply them by N to get the total. Next, let's compute the average energy of each oscillator: $\langle E \rangle = U = -1/2 \beta Z \langle \ln(Z) \rangle = U = \langle \ln(Z) \rangle / \beta$ where $\beta = 1/kT$. Therefore, $U = -2 \sinh(\epsilon / kT) / \cosh(\epsilon / kT)^2$. The heat capacity of one oscillator is then $C_V = \partial U / \partial T = -2 \sinh(\epsilon / kT) / \cosh(\epsilon / kT)^2$. The heat capacity of the entire solid is then given by $C_V = 3N \langle \ln(Z) \rangle / \beta$, where the total number of degree of freedom of the solid is three (for the three directional degree of freedom) times N . The Debye model predicts a linear function of the ratio T / D , where D is the Debye temperature. [2] Hence, the Einstein crystal model predicts that the energy and heat capacities of a crystal are universal functions of the dimensionless ratio T / D . Similarly, the Debye model is found by quantizing the normal modes of the solid in the same way the Einstein suggested. Then the frequencies of the waves are not all the same, and the specific heat goes to zero as a T^3 power law, which matches experiment. This modification is called the Debye model, which appeared in 1912. See also Kondo theory of solids References Mandl, F. (1986) [1971]. Statistical Physics (2nd ed.). Chichester-New York-Brisbane-Toronto-Singapore: John Wiley & Sons. ISBN 978-0471915331. Rogers, Donald (2005). Einstein's other theory: the Planck-Bose-Einstein theory of heat capacity. Princeton University Press. p. 73. ISBN 0-691-11826-4. External links Zelený, Enrique. The Wolfram Demonstrations Project - Einstein Solid. Retrieved 2016-03-18.. Retrieved from "

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