

PREDICTIONS FOR COOLING A SOLID TO ITS GROUND STATE

BY

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Abstract. A major goal of quantum computing research is to drain all quanta (q) of thermal energy from a solid at a positive temperature $T_0 > 0$, leaving the object in its ground state. In 2010 the first complete success was reported when a quantum drum was cooled to its ground state at $T_0 = 20\text{mK}$. However, current theory, which is based on the Bose-Einstein equation, predicts that temperature $T \rightarrow 0$ as $q \rightarrow 0$. We prove that this discrepancy between experiment and theory is due to previously unobserved errors in low temperature predictions of the Bose-Einstein equation. We correct this error and derive a new formula for temperature which proves that $T \rightarrow T_0 > 0$ as $q \rightarrow 0$. Simultaneously, the energy decreases to its ‘supersolid’ ground state level as $q \rightarrow 0^+$. For experimental data our temperature formula predicts that $T_0 = 9.8\text{mK}$, in close agreement with the 20mK experimental result. Our results form a first step towards bridging the gap between existing theory and the construction of useful quantum computing devices.

1. Background. In 2009-2010 Park and Wang [7], Schliesser et al [12], Groblacher et al [4], and Rocheleau et al [10] used laser cooling techniques to cool solids to temperatures where the number of remaining quanta (q) are 63, 37, 30 and 4, respectively. In 2010 O’Connell et al [6] achieved complete success in reducing the number of quanta in a quantum drum to zero at $T_0 = 20\text{mK}$. The key to their breakthrough was to use a ceramic wafer whose natural frequency, 6GHz ., is much higher than frequencies in previous studies. In 2011 Teufel et al [14, 15] reduced the number of quanta in a drumlike membrane to ‘less than one.’ They claim that their device remains in the ground state for 100 microseconds, significantly longer than the 6 nano second result in [6].

Theoretical investigations [14, 15] have focused on the assumption that the Bose-Einstein equation

$$q = \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1} \quad (1.1)$$

for a single atom represents the behavior of the entire solid. Here k is Boltzman’s constant, h is Planck’s constant, ν is frequency and $T > 0$ is temperature. In particular,

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a major component of the analysis by Teufel et al [14, 15] is crucially dependent on two well known predictions of the Bose-Einstein equation:

(**P**₁) Thermal energy is present at every positive temperature.

(**P**₂) $T \rightarrow 0$ as $q \rightarrow 0$.

The discrepancy between the experimental results of O'Connell et al [1] and theoretical predictions (**P**₁)-(**P**₂) clearly demonstrates that, as the quanta of energy are drained from a solid, the behavior of temperature is poorly understood.

The first step in resolving the discrepancy between experiment and theory is to define the limiting value of temperature by

$$T_0 = \lim_{q \rightarrow 0^+} T.$$

Our most important theoretical advance (see Theorem 2.1) is the following:

We derive a new formula for temperature of a solid which proves that $T_0 > 0$, and therefore predictions (**P**₁)-(**P**₂) of the Bose-Einstein equation are false.

To prove this claim we analyze the Einstein model of a solid [2]. The Einstein model is based on the following assumptions:

(**A**1) Each of the N atoms in the lattice of the solid is a 3D quantum harmonic oscillator, and $q > 0$ quanta of energy have been added to the lattice.

(**A**2) Each atom is attached to a preferred position by a spring.

(**A**3) The oscillators have the same frequency $\nu > 0$.

In agreement with the single atom model, the Einstein model assumes monochromatic vibrations of the atoms making up the solid. Thus, the Einstein model is the natural extension from the single atom model to an entire solid.

In 1907 Einstein derived his classical formula for specific heat, at constant volume, of a solid which satisfies (**A**1)-(**A**2)-(**A**3):

$$C_V = 3N_A k \left(\frac{\epsilon}{kT} \right)^2 \frac{\exp(\frac{\epsilon}{kT})}{(\exp(\frac{\epsilon}{kT}) - 1)^2}, \quad 0 < T < \infty, \quad (1.2)$$

where N_A is Avogadro's number, $\epsilon = h\nu$ is the quantum of energy, and ν is frequency. Formula (1.2) has the following basic property: let $\frac{\epsilon}{k} > 0$ be fixed. Then (see Figure 1)

$$C_V \text{ is well defined for all } T > 0 \text{ and } \lim_{T \rightarrow 0^+} C_V = 0. \quad (1.3)$$

Property (1.3) is widely quoted in textbooks and reference books in the statistical mechanics, thermal physics and modern physics literature (e.g. see Prathia [9], p. 175, Schroeder [12], p. 309, or Tipler and Llewellyn [16], p.347). Our second most important advance is to prove that both parts of (1.3) are *false*.

To prove the claims made above, we reexamine the details of the derivation of formula (1.2). There are two standard methods to derive (1.2). We follow the micro canonical ensemble approach [9, 13], since it is based on standard statistical mechanics principles which precisely describe how temperature and energy change as the quanta are drained from the solid. The second method, the macro canonical approach, uses partition

functions [3, 9] which do not immediately show the effect of decreasing the number of quanta. However, the details of their derivation do show such effects.

The first step is to show how expressions for internal energy, entropy and temperature lead to the underlying Bose-Einstein equation. Secondly, we prove that the discrepancy between experiment and current theory is due to previously unobserved mathematical errors that arise in the Bose-Einstein equation as $q \rightarrow 0^+$. We then present our approach to resolve these errors. Our results are stated in Theorem 2.1.

The possible energy states of the atoms are $E_k = \epsilon \left(n_k + \frac{1}{2} \right)$, $1 \leq k \leq N' = 3N$. Thus, the total internal energy is

$$U = \sum_{k=1}^{N'} \epsilon \left(n_k + \frac{1}{2} \right) = \epsilon q + U_0, \quad (1.4)$$

where $q = \sum_{k=1}^{N'} n_k$ is the number of quanta and $U_0 = \frac{N'\epsilon}{2}$ is ground state energy.

The Boltzman formula for entropy is $S = k \ln(W)$, where W is the number of ways that q quanta can be distributed over $N' = 3N$ degrees of freedom. Thus, $W = \frac{(q+N'-1)!}{q!(N'-1)!}$ and $S = k \ln \left(\frac{(q+N'-1)!}{q!(N'-1)!} \right)$. Therefore,

$$S = k (\ln((q + N' - 1)!) - \ln(q!) - \ln((N' - 1)!)). \quad (1.5)$$

The standard statistical mechanics approach to simplify (1.5) is to use Stirling's approximation $\ln(M!) = M \ln(M) - M$, $M \gg 1$ [9, 13]. Applying Stirling's approximation to (1.5) when $q \gg 1$ and $N' \gg 1$ gives

$$S = k ((q + N' - 1) \ln((q + N' - 1)) - q \ln(q) - (N' - 1) \ln(N' - 1)), \quad (1.6)$$

Temperature and specific heat satisfy

$$\frac{1}{T} = \frac{\partial S}{\partial U} \text{ and } C_V = \frac{1}{n} \frac{\partial U}{\partial T}, \quad (1.7)$$

where $n = \frac{N}{N_A}$ (moles). It follows from (1.4), (1.6) and (1.7) that

$$\frac{1}{T} = \frac{dS}{dq} \frac{dq}{dU} = \frac{k}{\epsilon} \ln \left(\frac{q + N' - 1}{q} \right). \quad (1.8)$$

An inversion of (1.8) gives the Bose-Einstein equation for the solid:

$$q = \frac{N' - 1}{e^{\frac{\epsilon}{kT}} - 1}. \quad (1.9)$$

Next, ignore -1 in the numerator since $N' \gg 1$, substitute (1.9) into (1.4), and get

$$U = \frac{\epsilon N'}{e^{\frac{\epsilon}{kT}} - 1} + \frac{N'\epsilon}{2}. \quad (1.10)$$

Finally, set $N' = 3N$, $n = \frac{N}{N_A}$, and combine (1.10) with $C_V = \frac{1}{n} \frac{dU}{dT}$. This gives Einstein's specific heat formula (1.2).

2. The Mathematical Error And Its Resolution. It follows from the Bose-Einstein equation (1.9) that

$$T_0 = \lim_{q \rightarrow 0^+} T = 0. \quad (2.1)$$

Equations (1.9) and (2.1) predict, in agreement with predictions **(P₁)-(P₂)** of the single atom model, that thermal energy is present in the solid at every positive temperature, and that $T \rightarrow 0$ as the quanta are drained from the solid. However, (1.9) and (2.1) are mathematically illegitimate since their derivations are directly dependent on the Stirling approximation $\ln(q!) = q \ln(q) - q$, which is accurate when $q \gg 1$, but rapidly loses accuracy as $q \rightarrow 0^+$: the relative error is 13 percent at $q = 10$, and 188 percent at $q = 2$. Indeed, the term $q \ln(q) - q$ is actually negative at $q = 1$ or $q = 2$. To correct this unacceptable loss of accuracy, our approach is to return to formula (1.5) for S , and replace each term of the form $\ln(M!)$ with the *exact* value $\ln(M!) = \ln(\Gamma(M+1))$, where Γ is the Gamma function. This transforms (1.5) into

$$S = k (\ln(\Gamma(q+N')) - \ln(\Gamma(q+1)) - \ln(\Gamma(N'))) \quad \forall q \geq 0. \quad (2.2)$$

In Theorem 2.1 we use (2.2) to derive new expressions for T , U and C_V which are completely accurate over the *entire* range $0 < q < \infty$.

THEOREM 2.1. Let $\epsilon > 0$ and $N' \gg 1$ be fixed. Temperature is given by

$$T = \frac{\epsilon}{k} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right)^{-1} > 0 \quad \forall q \geq 0. \quad (2.3)$$

T is an increasing function of q . Its lowest value is

$$T_0 = \lim_{q \rightarrow 0^+} T = \frac{\epsilon}{k} \left(\frac{\Gamma'(N')}{\Gamma(N')} + \gamma \right)^{-1} > 0, \quad (2.4)$$

where γ is Euler's constant.

Energy, U , is an increasing function of q , and satisfies

$$\lim_{q \rightarrow 0^+} U = N' \frac{\epsilon}{2} = \text{Ground State Energy}. \quad (2.5)$$

Specific heat is given by

$$C_V = -\frac{k}{n} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right)^2 \left[\frac{d}{dq} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right) \right]^{-1} > 0 \quad \forall q \geq 0. \quad (2.6)$$

C_V is an increasing function of q . The lowest value of C_V is positive, and is given by

$$C_0 = \lim_{q \rightarrow 0^+} C_V = -\frac{k}{n} \left(\frac{\Gamma'(N')}{\Gamma(N')} + \gamma \right)^2 \left[\frac{d}{dq} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right) \Big|_{q=0} \right]^{-1} > 0. \quad (2.7)$$

The proof of Theorem 2.1 is given in the Appendix. We make the following conclusions:

(I) Minimum temperature and energy. It follows from (2.4) that temperature decreases to a *positive* value $T_0 > 0$ as $q \rightarrow 0^+$, and cannot go lower. This result, which

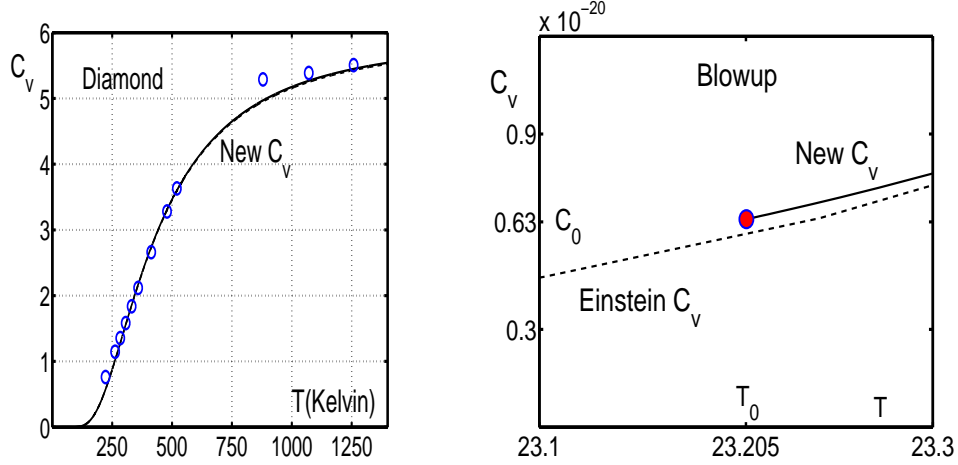


FIG. 1. Left panel: Einstein's C_v function (1.2) vs. T for diamond: data from [3], frequency $\nu = 2.727 \times 10^{13}$. Superimposed is the new C_v function (2.6) Right panel: blowup showing both functions vs T when $23.1 < T < 23.3$ The red dot corresponds to $T_0 = 23.205$, the positive temperature where this solid reaches its ground state.

overturns predictions (\mathbf{P}_1) - (\mathbf{P}_2) of the Bose-Einstein equation, is surprising and unexpected since Bose-Einstein equations have not previously been known to give mathematically erroneous predictions. Furthermore, as $q \rightarrow 0^+$ property (2.5) shows that energy decreases to the 'supersolid' ground state level where all atoms in the lattice have the same energy $\epsilon = h\nu$. Thus, at $T = T_0$ quantum effects are expected, e.g. superposition of states [8] or possibly superfluidity [5].

(II) Comparison with experiment. To test formula (2.4) we use data from O'Connell et al [6]: frequency = 6GHz and $N \approx 1$ trillion atoms. Thus, $\epsilon = 3.98 \times 10^{-24}$, $N' = 3N \approx 3 \times 10^{12}$, and formula (2.4) gives

$$T_0 \approx 9.8mK, \quad (2.8)$$

which closely agrees with the 20mK experimental result of O'Connell et al [6].

(III) Diamond. When $n = 1$ mole, (2.4) predicts that T_0 depends only on frequency:

$$T_0 = 8.508 \times 10^{-13}\nu, \quad 0 < \nu < \infty. \quad (2.9)$$

Formula (2.9) shows that T_0 can be large, potentially reaching room temperature, when ν is large. When $\nu = 2.726 \times 10^{13}$, the value given by Einstein [3] for diamond, (2.9) gives (see Figure 1, right panel)

$$T_0 = 23.2K$$

This high value is expected since diamond is extremely hard, hence its natural frequency is high. This prediction, which is easily tested, is in agreement with the results of O'Connell et al [6], which show that a high frequency solid more easily reaches its ground state at a positive temperature.

(IV) New Experiment. Recently, Romero-Isart et al [11] proposed an interesting experiment to extend the ground breaking results of O’Connell et al [6]. Their proposal is to cool a sphere containing millions of atoms to its ground state, where they predict it will exhibit the quantum property of superposition of states. Our temperature estimates in Theorem 2.1 may provide valuable insights for the design of such experiments.

(V) Specific heat. We conclude from (2.6)-(2.7) that C_v decreases to a positive value $C_0 > 0$ as $q \rightarrow 0^+$, and cannot go lower (Figure 1, right panel). This is our second most important theoretical prediction since it overturns (1.3), the widely acclaimed principle that “ C_v is well defined for all $T > 0$, and $\lim_{T \rightarrow 0^+} C_v = 0$.”

(VI) The Debye Model. The 1913 Debye model of a solid extends Einstein’s assumption **(A3)** to include solids with variable frequencies in the lattice of atoms [1]. The Debye model is also well known to satisfy (1.3). However, a modification (not shown) of the techniques in this paper proves that $T_0 > 0$, and therefore property (1.3) is not true for Debye’s model.

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3. Appendix. Proof of Theorem 2.1. The first step is to prove crucial properties of entropy, S , and internal energy, U . We conclude from (2.2) and (1.4)

$$\frac{dS}{dq} = k \left(\frac{\Gamma'(q + N')}{\Gamma(q + N')} - \frac{\Gamma'(q + 1)}{\Gamma(q + 1)} \right) \quad \text{and} \quad \frac{dU}{dq} = \epsilon \quad \forall q > 0. \quad (3.1)$$

Temperature. It follows from the fact that $\frac{1}{T} = \frac{\partial S}{\partial U}$, and (3.1) that

$$\frac{1}{T} = \frac{dS}{dq} \frac{dq}{dU} = \frac{k}{\epsilon} \left(\frac{\Gamma'(q + N')}{\Gamma(q + N')} - \frac{\Gamma'(q + 1)}{\Gamma(q + 1)} \right) \quad \forall q \geq 0. \quad (3.2)$$

This, together with the property

$$\frac{d}{dx} \left(\frac{\Gamma'(x)}{\Gamma(x)} \right) = \int_0^\infty \frac{te^{-xt}}{1 - e^{-t}} dt > 0 \quad \forall x > 0, \quad (3.3)$$

implies that

$$T = \frac{\epsilon}{k} \left(\frac{\Gamma'(q + N')}{\Gamma(q + N')} - \frac{\Gamma'(q + 1)}{\Gamma(q + 1)} \right)^{-1} > 0 \quad \forall q \geq 0. \quad (3.4)$$

This proves property (2.3).

Next, let ϵ, k and N' be held fixed in (3.4). Then the only way that T can increase, or decrease, is to change q . We claim that T is an increasing function of q . The first step in proving this claim is to differentiate (3.4). This gives

$$\frac{dT}{dq} = -\frac{\epsilon}{k} \left(\frac{\Gamma'(q + N')}{\Gamma(q + N')} - \frac{\Gamma'(q + 1)}{\Gamma(q + 1)} \right)^{-2} \frac{d}{dq} \left(\frac{\Gamma'(q + N')}{\Gamma(q + N')} - \frac{\Gamma'(q + 1)}{\Gamma(q + 1)} \right) \quad \forall q \geq 0. \quad (3.5)$$

To prove that T is an increasing function of q , we need to show that the right side of (3.5) is positive when $q \geq 0$. The second term is negative since

$$\frac{d^2}{dx^2} \left(\frac{\Gamma'(x)}{\Gamma(x)} \right) = - \int_0^\infty \frac{t^2 e^{-xt}}{1 - e^{-t}} dt < 0 \quad \forall x > 0. \quad (3.6)$$

Therefore, the right side of (3.5) is positive, hence

$$\frac{dT}{dq} > 0 \quad \forall q \geq 0. \quad (3.7)$$

Thus, T is an increasing function of q . From this and (3.4) we conclude that the lowest possible value of temperature is positive, and is given by

$$T_0 = \lim_{q \rightarrow 0^+} T = \frac{\epsilon}{k} \left(\frac{\Gamma'(N')}{\Gamma(N')} - \frac{\Gamma'(1)}{\Gamma(1)} \right)^{-1} = \frac{\epsilon}{k} \left(\frac{\Gamma'(N')}{\Gamma(N')} + \gamma \right)^{-1} > 0, \quad (3.8)$$

since $\Gamma'(N') > 0$, $\Gamma(N') > 0$, $\Gamma(1) = 1$ and $\Gamma'(1) = -\gamma$.

Energy. It follows from (1.4) that internal energy, U , is given by

$$U = \epsilon q + U_0, \quad (3.9)$$

where $U_0 = \frac{N'\epsilon}{2}$ is ground state energy, and $q = \sum_{k=1}^{N'} (n_k + \frac{1}{2})$ is the total number of quanta of thermal energy. We conclude from (3.9) that

$$\lim_{q \rightarrow 0^+} U = \frac{N'\epsilon}{2} = \text{Ground State Energy.} \quad (3.10)$$

This proves property (2.5).

Specific Heat. We conclude from (1.7) and (3.1) that

$$C_V = \frac{1}{n} \frac{\partial U}{\partial T} = \frac{1}{n} \frac{\partial U}{\partial q} \frac{\partial q}{\partial T} = \frac{\epsilon}{n} \frac{\partial q}{\partial T}. \quad (3.11)$$

It follows from (3.5) and (3.7) that

$$\frac{\partial q}{\partial T} = -\frac{k}{\epsilon} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right)^2 \left[\frac{d}{dq} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right) \right]^{-1} > 0 \quad \forall q \geq 0. \quad (3.12)$$

Combining (3.11) and (3.12) gives

$$C_V = -\frac{k}{n} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right)^2 \left[\frac{d}{dq} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right) \right]^{-1} > 0 \quad \forall q \geq 0. \quad (3.13)$$

From (3.13) it follows that C_V is an increasing function of q . Thus, the lowest possible value of specific heat is found by letting $q \rightarrow 0^+$. This gives

$$\lim_{q \rightarrow 0^+} C_V = C_0 = -\frac{k}{n} \left(\frac{\Gamma'(N')}{\Gamma(N')} + \gamma \right)^2 \left[\frac{d}{dq} \left(\frac{\Gamma'(q+N')}{\Gamma(q+N')} - \frac{\Gamma'(q+1)}{\Gamma(q+1)} \right) \Big|_{q=0} \right]^{-1} > 0. \quad (3.14)$$

This proves property (2.7). The proof of Theorem 2.1 is now complete.