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A Schottky-Like Anomaly in Systems with a Finite Number of Layers

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A Schottky-like anomaly is found in systems with a *finite* number of layers for both classical and quantum particles. Unlike the usual scenario for the anomaly, there is no excitation gap in these systems. We analyze its dependence on the layer number and the hopping amplitude between neighbouring layers.

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I. INTRODUCTION

In high-temperature superconducting thallium or bismuth oxide[1] the superconducting transition temperature, T_c, is observed to increase with the number of Cu-0 layers up to three layers. Theoretically we know that, in the absence of coupling between the layers or with ions outside of the layer, a single layer is forbidden by the Mermin-Wagner theorem [2] to exhibit a finite T_c. According to Anderson [3], spin and charge degrees of freedom for each electron are separated in the Cu-0 plane into the so-called spinon and holon excitations, and holons are paired into a coherent state below T_c. Since only electrons can hop between layers, it becomes energetically favourable for the electrons to form pairs before hopping (which thus enhances and gives a finite T_c) in order not to break the holon pairs.

It is natural to ask whether a similar enhancement occurs for the Bose condensation in multilayer systems. Since the condensation temperature $T_B = 0$ for an ideal Bose gas in a single layer, we need to determine first how many layers n there are and how strong the hopping amplitude betweecn neighbouring layers t is required to produce a finite T_B before discovering how they enhance it. For $n = \infty$, the answer is immediate because we can treat the system as in a 3-D continuum and expand [4] the kinetic energy in the discrete direction $2t \cos ka$, where a is the spacing between neighbouring layers, into the free particle form with an effective mass $\hbar^2/2ta^2$. It is then easy to show that

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$$T_{\mathrm{B}} \approx \hbar^{\frac{4}{3}} \left(\frac{N}{mA} \right)^{\frac{2}{3}} t^{\frac{1}{3}} , \tag{1}$$

where $\frac{N}{A}$ and m are the boson density and the boson mass in the layer. Naively, one may expect a critical and finite value for n and t beyond which the system crosses over from two to three-dimensional behaviour. This is wrong however, because, as long as n is finite, the density of states that most bosons experience remains that of two dimensions at temperatures lower than the level difference [5] in the discrete direction. In other words, condensation can not occur at finite temperatures for an ideal boson gas, unless n is strictly infinite.

For systems with a finite number of layers, the specific heat, $C_V(T)$, is found to exhibit an anomalous peak for both classical and quantum particles (see Fig. 1). Having ruled out the possibility of a Bose condensation (this is naturally not the cause since the anomaly is not unique to bosons), we identify this anomaly to be of the Schottky type (there is no Kosterlitz-Thouless transition [6] because these particles are assumed to be ideal). A Schottky anomaly, see Fig. 2(a), is generally observed in systems with an excitation gap A and obeys [7]

$$C_V(T) = \left(\frac{\Delta}{k_{\mathrm{B}} T} \right)^2 e^{\Delta / k_{\mathrm{B}} T} (1 + e^{\Delta / k_{\mathrm{B}} T})^{-2} .$$

In multilayer systems, the discrete direction gives rise to discrete energy levels [5] which, however, are superimposed on the continuous 2-D spectrum from the layer (which wipes

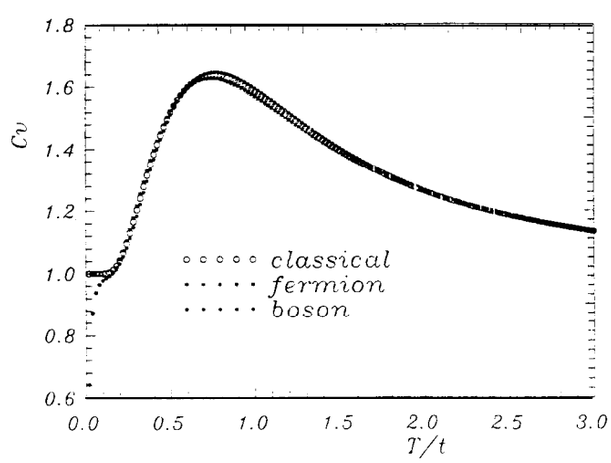
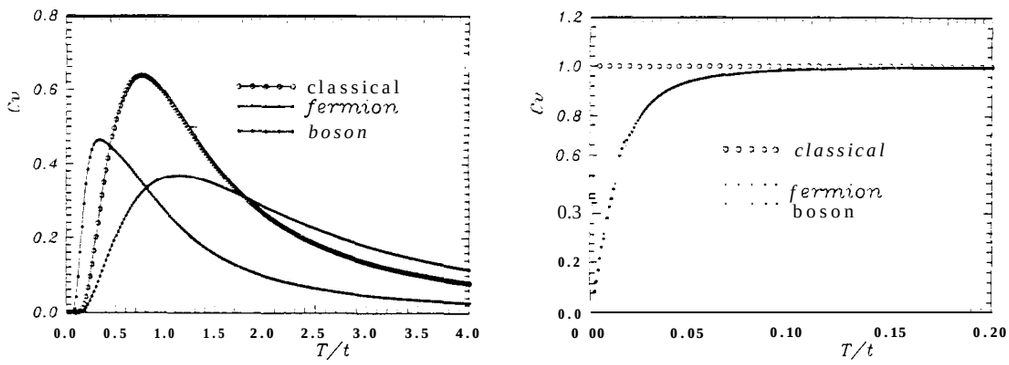


FIG. 1. $C_V(T)$ for a three-layer system with a hopping amplitude $t = 100$ Ii, particle density $N/A = 5.3 \times 10^{13} \mathrm{m}^{-2}$ per layer and the particle mass of a bare electron. Note that at low temperatures $C_V \to 1$ for classical particles while $C_V \to 0$ for quantum particles.



(a) (b)

FIG. 2. Temperature dependence of the specific heat for (a) two particles at three discrete energy levels, $E_\ell = 2t\cos\left(\frac{\ell\pi}{4}\right)$ where $\ell = 1, 2, 3$ and $t = 100$ K and (b) a continuous 2-D gas with $N/A = 5.3 \times 10^{13}\,\mathrm{m}^{-2}$. The boson line is slightly above the fermion line in (b).

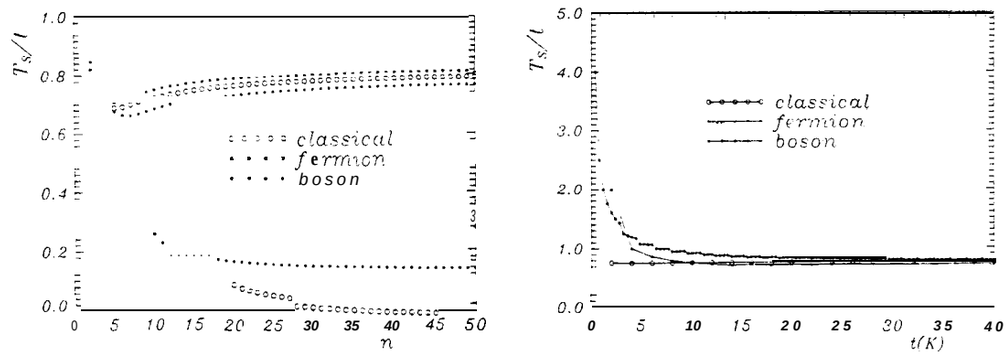
out the excitation gap). Fortunately, for classical particles, these two spectra are separable for the internal energy

$$U = \frac{\sum_{k_x,k_y}\sum_{k_z}[E_1(k_x,k_y)+E_2(k_z)]e^{-\beta[E_1(k_x,k_y)+E_2(k_z)]}}{\sum_{k_x,k_y}\sum_{k_z}e^{-\beta[E_1(k_x,k_y)+E_2(k_z)]}}$$

$$= \frac{\sum_{k_x,k_y}E_1(k_x,k_y)e^{-\beta E_1(k_x,k_y)}}{\sum_{k_x,k_y}e^{-\beta E_1(k_x,k_y)}} + \frac{\sum_{k_z}E_2(k_z)e^{-\beta E_2(k_z)}}{\sum_{k_z}e^{-\beta E_2(k_z)}}.$$

This proves that the origin of the anomaly is from the discrete direction and of the Schottky type (remember that the 2-D spectrum gives the temperature-independent Dulong-Petit value). However this separation is not possible for quantum particles, and our same identification is based partly on the qualitative resemblance between Fig. 1 and Figs. 2(a) and 2(b) combined.

Figure 3 shows the dependence of T_S, the temperature where the anomaly occurs, on n and t for systems with a finite number of layers. For quantum particles, roughly by adding the contributions of Figs. 2(a) and (b), we expect the T_S of Fig. 2(a) to increase (because the derivative in Fig. 2(b) is positive definite) by an amount determined by $\hbar^2 N/mA$. This increase in T_S is observed for fermions and classical particles but not for bosons. Note that there are two peaks, i.e., two T_S values in Fig. 3(a), at large n, except for fermions. We believe the lower value for bosons is due to the tendency towards a Bose condensation, which is why it only occurs at large n when the system is more "three-dimensional". We check this for various t-values and find $T_S/t \propto 1/t^{2/3}$ as predicted by Eq. (1) for the condensation



(a) (b)

FIG. 3. For a multilayer system with $N/A = 5.3 \times 10^{13}\,\mathrm{m}^{-2}$ the temperature where the Schottky-like anomaly occurs, T_S, is normalized by the hopping amplitude t and plotted as a function of (a) the layer number n, with t=100K, and (b) t for three layers.

temperature of an infinite multilayer system. Fig. 4 shows the dependence of their relative size on n. We can see that the Schottky-like peak dominates at small n, while the other dominates at large n. The convergence of all the lines at large t in Fig. 3(b) is due to the

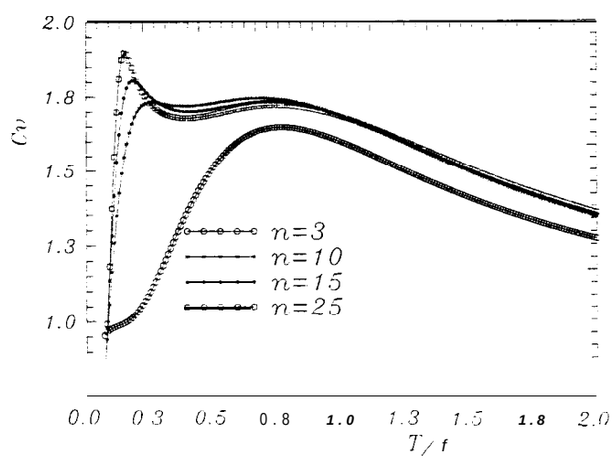


FIG. 3. $C_V(T)$ for ideal bosons in a multilayer system with the same parameters as in Fig. 1 for various layer numbers. Note that two peaks appear at large n. The first one is due to the tendency towards Bose-Einstein condensation, and the second is the Schottky-like anomaly.

fact that the t-dependence of $\frac{T_S}{t}$ is through the unitless variable $\frac{\hbar^2 N/mA}{t}$, and increasing t is equivalent to decreasing N/mA. As we know, when quantum particles are dilute, their quantum behaviour is diminished. Similarly, the convergence of the higher T_S values in Fig. 3(a) can be understood.

To discuss the origin of the second lower T_S value for classical particles in Fig. 3(a), we only need to concentrate on the discrete spectrum. Fig. 5 shows the large n behaviour of $C_V(T)$ for systems with discrete energy levels, $E_\ell = 2t\cos\frac{\ell\pi}{n+1}$ where $\ell = 1, \cdots, n$. Note that a small peak appears before the Schottky-like anomaly for classical particles and fermions. We check the n-dependence of the temperature at which this peak occurs and obtain a very good $1/n^2$ behaviour. We believe this is an artifact of the form of the energy levels. The reason being that in the case of classical particles, if n is infinite, $C_V(T \to 0)$ approaches [8] $1/2$ – the Dulong-Petite value instead of the thermally activated form $\exp(-\Delta/T)$, where $\Delta \approx t/n^2$ for a finite n. Therefore we can imagine (as Fig. 5 also shows) that, when n is large, C_V will increase sharply from 0 at $T = 0$ to above $1/2$ at about $T \sim t/n^2$, when the excitation gap is thermally smeared out. Presumably this sharp rise renders the small bump at $T \sim t/n^2$ before the Schottky-like peak. Next is the case of fermions. Note that the level difference is the largest at $\ell \sim n/2$ for $E_\ell = 2t\cos\frac{\ell\pi}{n+1}$ and that the levels are less than half-filled when n is large. Since fermions distribute more outwards in energy, their relevant energy scale (from the level difference) and corresponding T_S will be larger than those of classical particles. Fig. 5 shows that $C_V(T)$ rises more dramatically than for

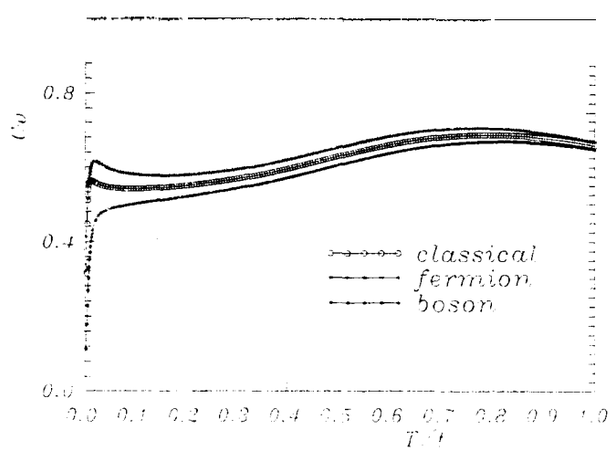


FIG. 5. $C_V(T)$ for two particles with discrete energy levels, $E_\ell = 2t\cos(\frac{\ell\pi}{n+1})$ where $t = 100$ K, $n = 50$, and $\ell = 1, \cdots, n$.

classical particles. We ascribe this to the fact that, when levels are less than half-filled, less and less thermal energy is required to excite the next deep occupied state.

In conclusion, we find a Schottliy-like anomaly in systems with a finite number of layers for both classical and quantum particles. Unlike the usual scenario for the anomaly, there is no excitation gap in these systems. Its dependence on the layer number and hopping amplitude between neighbouring layers is analyzed. The tendency towards Bose-Einstein condensation is believed to make a second peak for bosons when the layer number is large.

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[4] Since bosons occupy mainly the small k states at low temperatures, we can expand the energy about the $k = 0$ state.

[5] If we assume a constant hopping amplitude t between neighbouring layers, the eigenenergies in the discrete direction are nothing but the eigen-modes of a series of springs with fixed boundary conditions: $E_\ell = 2t\cos(\frac{\ell\pi}{n+1})$ where ℓ is an integer ranging from 1 to n. See J. B. Marion, *Classical Dynamics of Particles and Systems* (Academic, New York, 1970).

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[7] See R. K. Pathria, *Statistical Mechanics* (Pergamon, New York, 1972), p. SS.

[8] When n $\gg$ 1, $\sum_{\ell=1}^{n} f(\cos(\frac{\ell\pi}{n+1}))$ can be written as $\frac{n}{\pi}\int_0^\pi f(\cos\theta)d\theta$ and the partition function for classical particles can be identified as the modified Bessel function, $I_0(2\beta t)$, times n.