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Non-Extensive Statistics and High Temperature Superconductivity

by

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Abstract

The theoretical understanding of high temperature superconductivity remains one of the most important unanswered questions in contemporary condensed matter physics. A wealth of experimental data accumulated since the discovery of this phenomenon [1] has set strict guidelines as to what a successful theory must incorporate. This has been complemented with an equally large yet incomplete body of theoretical interpretations of the problem. In this thesis a generalized formulation of the BCS[2] theory of superconductivity, based on a non-extensive statistics suggested by Tsallis [3], is proposed. The treatment is purely two-dimensional in accordance with the large anisotropy in the conduction states of all known high temperature superconductors (high T_c's). This is justifiable as the loss of phase coherence due to fluctuations in lower dimensional superconductors, no longer persists in this generalized formulation, except in the limit where Boltzmann-Gibbs statistics are recovered. A generalization of the

BCS universality condition emerges in the form $\frac{2\Delta_0}{qk_BT_c} \sim 3.52$ where q measures the degree of non-extensivity of the system. Many other characteristic physical properties of high T_c superconductors can also be described satisfactorily in this formulation.

Nie-Ekstensiewe Statistiek en Hoë Temperatuur Supergeleiers

deur

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Fakulteit: Natuur- en Landbouwetenskappe

Departement: Fisika

Graad: Magister Scientiae

Uittreksel

'n Volledige teoretiese begrip van hoë temperatuur supergeleiding is steeds een van die mees belangrike onopgeloste vrae in hedendaagse veelligaam fisika. 'n Magdom eksperimentele data versamel sedert die ontdekking van die verskynsel [1] stel streng maatreëls waaraan 'n suksesvolle teorie moet voldoen. Hierdie word gekomplementeer met 'n ewe groot dog onvolledige liggaam van teoretiese interpretasies van die probleem. In hierdie tesis word 'n veralgemeende formulering van die BCS[2] teorie van supergeleiding gebaseer op 'n nie-ekstensiewe statistiese meganika soos voorgestel deur Tsallis [3], voorgelê. Die benadering is suiwer tweedimensioneel in ooreenstemming met die groot anisotropie van die geleidings toestande van alle bekende hoë temperatuur supergeleiers. Laasgenoemde is verantwoordbaar aangesien die verlies van fase koherensie a.g.v. fluktuasies in supergeleiers van laer dimensie, nie voorkom in die veralgemeende formulering nie, behalwe in die limiet waar Boltzmann-Gobbs

statistiek herstel word. 'n Veralgemening van die BCS universele voorwaarde word verkry in die vorm $\frac{2\Delta_0}{qk_BT_c} \sim 3.52$ waar q die graad van nie-ekstensiwiteit van die sisteem aandui. Vele ander fisiese eienskappe van die hoë temperatuur supergeleiers kan bevredigend beskryf word in hierdie formulering.

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Chapter 1

Introduction

The discovery of superconductivity in the copper oxides in 1986 [1] and the subsequent race for even higher critical temperatures (125K by 1993 [5, 6]) raised hopes for the application of superconducting phenomena at operating temperatures approaching room temperature. The inability of the Bardeen-Cooper-Schrieffer (BCS) model [2] to satisfactorily describe superconductivity in these materials, appears to indicate that we are dealing with a completely different class of superconductors.

Various theoretical models have since been proposed. Currently one of the most widely supported models is that of d-wave superconductivity [7, 8]. The basic idea of this model is that the large anisotropy of the crystal structure of all high temperature superconductors (high T_c's) leads to an anisotropy in the order parameter of the superconducting state. Typically this might resemble the symmetry of a d-wave orbital angular momentum e.g.

$$\Delta(\mathbf{k}) = \Delta_d \left[\cos\left(k_x a\right) - \cos\left(k_y a\right)\right] \tag{1.1}$$

where Δ is the d wave order parameter, $\mathbf{k}$ the wave vector and a the planar lattice spacing between Cu ions. The $\mathbf{k}$ dependence implies that the

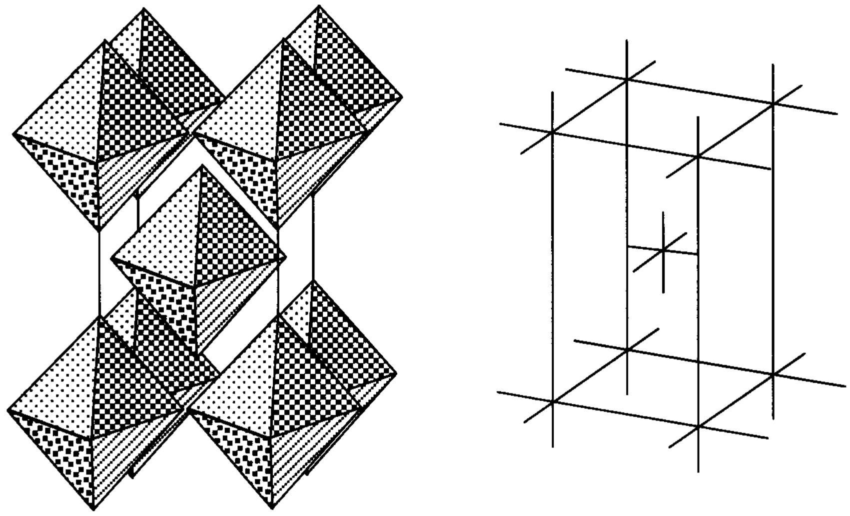

Figure 1.1: Basic crystal structure of $La_{2-x}Ba_xCuO_4$. One copper atom is situated at each point of the intersection of the lines in the frame structure on the right. They are each surrounded by six oxygen atoms forming the six corners of an octahedron as shown on the left. Lanthanum and barium atoms are not shown but lie between the planes of the octahedra.

gap does not have the same sign everywhere on the Fermi surface. In general, regions of opposite sign are separated by *nodal lines*. Some properties may in this model be predicted theoretically. Very strong evidence for this model exists, especially in the case of the so called heavy-fermion superconductors, such as UPt_3, UBe_3 and $CeCu_2Si_2$. However, many of the experiments designed to illustrate the gap-anisotropy in the cuprates, in fact rather support an s-wave model [9]. The coupling mechanism that would lead to such a model also remains a mystery. Therefore although its occurrence is a well established experimental fact, it appears as though d-wave coupling is neither a necessary nor sufficient condition for high-T_c superconductivity to occur.

Ultimately the physical properties of a material are based on the energy spectrum of excited states. It has been suggested that the occupation of these states in high T_c materials might obey 'para-statistics', an admixture of Bose and Fermi statistics [10, 11] since the exclusion principle applies very specifically to true Fermions only, and not necessarily to quasi-particles. In this case, however, the predicted universality condition is $\frac{2\Delta_0}{k_B T_c} < 3.52$ for all intermediate statistics, despite an exponential increase in the critical temperature.

Other more exotic models incorporate mechanisms such as non-phononic coupling or normal states of a different nature. Some examples are the polaron-bipolaron model [12], the resonating valence bond model [13], and the exciton model [14, 15]. Different degrees of success have been achieved in explaining specific aspects of high-T_c materials, but no inclusive model exists.

A number of characteristics must be incorporated in any such model. Certainly the main common denominator in all high-T_c materials is the large anisotropy in the crystal structure. Very typical is the body-centered tetragonal lattice of $La_{2-x}Ba_xCuO_4$ as illustrated in figure 1. Situated at each lattice point is a copper atom surrounded by six oxygen atoms forming the eight corners of an octahedron. Not shown in figure 1, are the lanthanum or barium atoms which lie in the spaces between octahedra of copper and oxygen. Also omitted is a small distortion tilting alternate octahedra left or right which makes the true structure orthorhombic. The result is conducting CuO_2 planes very nearly two dimensional in character. This can be seen in the large effective mass anisotropy in most high-T_c's e.g. $\sqrt{m_c^*/m_{ab}^*} = 52(1)$ in $HgBa_2Ca_3Cu_4O_{10}$ where m_c^* is the perpendicular and m_{ab}^* the in-plane effective masses respectively [16]. It is therefore reasonable to assume that lower dimensionality is essential for high critical temperatures and that arguably the 'ideal' high-T_c superconductor is purely two-dimensional in character. It is, however, well known that in BCS, a pure 2D model presents problems as the phase loses its coherence due to fluctuations [17]. This generally calls for at least a quasi-2D model.

Although the results of measurements on the superconducting gap are somewhat varied, there seems to be convergence towards a ratio of $\frac{2\Delta_0}{k_B T_c}$ equal to somewhere between 6 and 8 which is not consistent with the universal value of ~ 3.52 obtained for normal BCS superconductors. This is particularly so in the case of tunneling measurements [4, 18, 19, 20], where ratios as high as 8.9 have been measured in $La_{1.85}Sr_{0.15}CuO_4$ [21], but appears to contradict optical measurements [22, 23, 24] which seem to yield results closer to the BCS ratio for weak coupled superconductors. In the face of the apparent BCS behaviour of the tunneling currents, the violation of universality is difficult to understand.

Thirdly, experimental data suggests that the electronic contribution to the specific heat in cuprates does not exhibit the exponential form of normal weak coupled superconductors. It is rather of the linear form γT, where γ is of the order of a few mJ/mol·K^2. Magnetic properties of the high-T_c superconductors also differ appreciably from their normal counterparts, most notably in their very high upper critical fields. These fields are extrapolated to be of the order of tens or hundreds of Teslas and are too large to be attained with current technology. Furthermore it should also be noted that all high-T_c superconductors are of type II.

One of the strongest arguments for the phonon coupling scheme of the BCS model is the existence of an isotope effect. It was observed in 1950 [25] that the critical temperature scales very nearly as the square root of the isotopic mass of the crystal. In cuprate materials, where there is a strong doping dependence of the isotope effect, this requires some additional consideration. In optimally doped materials the effect is often strongly suppressed (T_c may scale as a power $\alpha = 0.1$ of the mass), whereas in overdoped or underdoped materials it might be more prevalent, with the scaling in some cases even exceeding $\alpha = 0.5$ [26].

Recently in statistical mechanics there has also been interest in a generalization of Boltzmann-Gibbs (BG) statistics to a non-extensive form proposed by Tsallis[3] in which the former is recovered in an appropriate limit. The formalism has had considerable success in providing an appropriate mathematical framework for dealing with physical systems with long-range interactions. Very good results have been obtained in relation to the so-called stellar "polytropes" [27] where the usual Boltzmann distribution functions yield unphysical results. A variety of other applications have also been considered such as turbulence in pure-electron plasma [28], the dynamic linear response for nonextensive systems [29], Lévy like anomalous diffusions [30], the solar neutrino problem [31] and long-range fluid and magnetic systems [32]. In addition many well-known theorems and principles have been formulated in generalized form, for example, Ehrenfest's theorem [33], von Neumann's equation [34], Jaynes' information theory duality [33], Bogolyubov's inequality [35] and others.

In this thesis we propose and motivate the possibility that the cuprate oxide materials have an inherent underlying non-BG like character responsible for their high-critical temperatures and other unusual properties. In order to preserve continuity of the free energy at the critical point, we conclude that it is a property of the material at lower temperatures and not some anomaly of the superconducting state. Our suggestion is that the s-wave BCS model is essentially correct in employing an effective weak coupling Hamiltonian that includes the kinetic energy of free electrons, along with a constant attractive potential between electrons of equal momentum and opposite spin [2]. The BCS ansatz in purely 2D form is used for the ground state, with a generalized form of the Fermi-distribution function [36] appearing at finite temperatures. We also show that such a 2D model is justified as the fluctuation-dissipation theorem is no longer valid in the Tsallis formalism [37]. The assumption that the coupling mechanism is purely phonon mediated, needs to be modified to obtain agreeable fits to experimental data, particularly in the case of very high temperature superconducting materials.

Chapter 2

Generalized Statistics

2.1 Motivation

The relevant question with regard to our proposed *modus operandi* is, of course, why the Tsallis formulation should be appropriate for the high-T_c's. The Tsallis entropy was specifically postulated with non-extensive systems in mind. These include systems having (i) long range interactions (ii) long term microscopic memory or (iii) fractal boundary conditions in space-time. If any one of these conditions apply, BG statistics are known to fail.

A very compelling argument can be found from a consideration of the electronic specific heat. The more exotic coupling methods mentioned above, may certainly have the effect of removing problems indirectly related to the BCS-Hamiltonian, such as the lattice instabilities predicted by Migdal [38]. The experimental evidence of an energy gap, however, requires an energy spectrum for the total energy of excitations, of the form

$$E_k^2 = \varepsilon_k^2 + \Delta^2, \tag{2.1}$$

where ε is the excitation energy and Δ the energy gap, independent of any proposed model. If one is to believe experimental evidence, Δ in (2.1) is independent of the wave number $\mathbf{k}$ and contrary to the d-wave model, the pairing is s-wave. Assuming a Fermi distribution, the electronic specific heat capacity (C) at temperatures $kT \ll \Delta$, can be shown to have the following form [39]

$$C \sim \frac{e^{-\frac{\Delta_0}{kT}}}{T^{\frac{3}{2}}} \tag{2.2}$$

One is therefore obliged to contend with an exponential form of the heat capacity in any s-wave pairing model that relies on the Fermi distribution function used in BG statistical mechanics. One way to circumvent this is to introduce a different distribution function.

It should be remembered that the most basic interaction in an electron gas is that of Coulomb repulsion. This interaction is of infinite range and may also introduce correlation effects. One example is the condensation of a true electron gas, of low enough density, into a *Wigner lattice* [40]. Very early attempts at explaining superconductivity, quite intuitively, but unsuccessfully, used the Coulomb potential as starting point [41, 42]. More recently models like those of Hubbard [43], describing contributions due to repulsion between electrons sharing an atomic orbital, have been applied to superconductivty. The condensation of electrons into its superfluid state is ultimately the result of an effective, attractive interaction. The extent of the effect of Coulomb repulsion might not be obvious and in spite of the fact that we do not explicitly take it into account in the effective interaction, we argue that it is precisely the effects of this long-range interaction which may render the system more suitable for description by generalized statistics.

2.2 Formulation of Generalized Statistics

The generalized entropy postulated by Tsallis [3] takes the form:

$$S_q = k\frac{\sum_{i=1}^{w}\{p_i - p_i^q\}}{q-1} \quad (q \in \Re) \tag{2.3}$$

where w is the total number of microstates in the system and p_i are the associated probabilities with $\sum_{i=1}^{w} p_i = 1$. q is a number that characterizes the degree of non-extensivity. It is straightforward to verify that the usual BG entropy is retrieved in the limit $q \to 1$

$$\begin{aligned} S_{BG} = \lim_{q\to 1} S_q &= k \lim_{q\to 1} \frac{1 - \sum_{i=1}^{w} p_i exp[(q-1)\ln p_i]}{q-1} \\ &= -k\sum_{i=1}^{w} p_i \ln p_i . \end{aligned} \tag{2.4}$$

The non-extensivity becomes apparent in the additivity rule

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B) \tag{2.5}$$

where A and B are two independent systems. It can also be shown that this entropy obeys the usual properties of concavity, equiprobability, positivity and irreversibility.

It can be demonstrated[3, 44] that S_q is an appropriate microscopic form of the entropy in statistical mechanics. We present some results to this end. Let us firstly state that by applying a variational principle to S_q, subject to the constraints $\sum_{i=1}^{w} p_i = 1$ and

$$U_q = \sum_{i=1}^{w} p_i^q \varepsilon_i \tag{2.6}$$

for the internal energy, it is possible to show [44] that a probability law applies for which

$$p_i = \frac{[1-\beta(1-q)\varepsilon_i]^{\frac{1}{1-q}}}{Z_q} \tag{2.7}$$

where Z_q is the partition function

$$Z_q = \sum_{i=1}^{w} [1 - \beta(1-q)\varepsilon_i]^{\frac{1}{1-q}}. \tag{2.8}$$

It is easily verified that

$$-\frac{\partial}{\partial \beta} \frac{Z_q^{1-q} - 1}{1-q} = U_q \tag{2.9}$$

which, in the $q \to 1$ limit, yields the standard expression $-\partial \ln Z_1 / \partial \beta = U_1$. Let us now Legendre transform the function $(Z_q^{1-q} - 1)/(1-q)$, which depends on β. Constructing $(Z_q^{1-q} - 1)/(1-q) + \beta U_q$ we find

$$\frac{Z_q^{1-q} - 1}{1-q} + \beta U_q = S_q \tag{2.10}$$

which again reproduces the standard relation $\ln Z_1 + \beta U_1 = S_1$ in the limit $q \to 1$. It immediately follows from (2.10) that

$$\frac{\partial S_q}{\partial U_q} = \frac{1}{\beta}. \tag{2.11}$$

Finally one can define a generalized free energy

$$F_q = U_q - T S_q \tag{2.12}$$

from which it straightforwardly follows

$$F_q = -\frac{1}{\beta} \frac{Z_q^{1-q} - 1}{1-q} \tag{2.13}$$

again recovering, for $q \to 1$, $F_1 = -(1/\beta) \ln Z_1$.

It is clear that the entire mathematical structure connecting standard statistical mechanics and thermodynamics is preserved within the Tsallis formulation.

Associated with equation (2.3) is a generalized Fermi distribution proposed by F. Büyükkiliç et al. [36]

$$f_q = \frac{1}{[1 + \beta(q-1)\epsilon_k]^{\frac{1}{q-1}} + 1}. \tag{2.14}$$

Once again the usual Fermi distribution of BG statistics is recovered in the limit $q \to 1$.

The validity of equation (2.14) has been the source of some dispute [45, 46], the problem being that one has to assume factorizability of the partition function to obtain this result. Büyükkiliç *et al* motivate this on the basis of the diluteness of a system and the consequent statistical independence of single particle states. We maintain that the inherent *independent quasi-particle* nature of the BCS-model allows for the same approximation to be made and we will henceforth assume (2.14) in our approach.

2.3 Interpretation of the Non-Extensive Parameter q

A very valid question is whether any physical interpretation can be associated with the parameter q. The simplest answer is that it is a measure of the degree of non-extensivity of a system, but this is not very satisfactory. Some authors have attempted to find generally applicable bounds on the value of q [47] and possible experimental tests have been proposed to identify systems as non-extensive [48]. All the latter might serve to elucidate the problem. Probably the most important step forward is the conclusion by Papa and Tsallis [49] that it is in fact possible to derive q from a knowledge of the microscopic dynamics of the system. A clearer picture is beginning to emerge (see also [50]) and it is certain that theorists will continue to address this matter in the future.

Chapter 3

The Fluctuation Dissipation Theorem

In the BG statistical mechanics, a simple relationship may be obtained between the canonical or grand canonical ensemble averages of commutators and anticommutators of two dynamical operators[51]. This relationship is often referred to as the fluctuation-dissipation theorem, since the anticommutator is used to describe time-dependent correlations or fluctuations in the system and the commutator is related to transport coefficients or dissipation[52, 53]. It is simply due to the fact that the Boltzmann factor or distribution function is exponential in nature and therefore factorizable. A consequence of this aforementioned theorem is to rigorously rule out the existence of superconductivity or superfluidity in one and two dimensions[54].

The approach to the high-T_c superconductor problem we shall propose in the next chapter, is based on the assumption that the "ideal" high T_c is purely 2D in nature. In light of the previous paragraph this needs to be justified. Unlike in the BG case, the generalized distribution function (2.14) we shall be using is not simply factorizable, except in the limiting case where BG statistics are recovered. Hence, as we shall show, the fluctuation-dissipation theorem as stated above no longer holds. This allows for the possibility of forming a condensate in two dimensions, provided these generalized statistics are realized.

To this end we require a generalized form of the Maxwell-Boltzmann distribution of an ideal gas [36]

$$f_q(\varepsilon_k) = [1 + \beta(q-1)(\varepsilon_k - \mu)]^{\frac{1}{q-1}} \tag{3.1}$$

where μ is the chemical potential. Now, with $\mu = 0$, consider the simplest form of canonical correlation function[51]

$$< \hat{A}(t)\hat{B}(t') >= Tr\{\hat{\rho}\hat{A}(t)\hat{B}(t')\} \tag{3.2}$$

where

$$\hat{\rho} \equiv \hat{\rho}_{q=1} \;=\; e^{-\beta\hat{H}}/Tr\{e^{-\beta\hat{H}}\} \tag{3.3}$$

$$=\; f_{q=1}(\hat{H})/Z_{q=1} \equiv f(\hat{H})/Z, \tag{3.4}$$

Z is the partition function and f_q is given by eq. (3.1). The spectral function for this correlation function may be written as

$$J_{AB}(\omega) \;=\; \int_{-\infty}^{\infty} e^{i\omega t} < \hat{A}(t)\hat{B}(0) > dt \tag{3.5}$$

$$=\; \int\int dEdE'\rho(E)2\pi\hbar\delta(E+\hbar\omega-E')j_{AB}(E,E') \tag{3.6}$$

where

$$j_{AB}(E,E') = Tr\{\delta(E-\hat{H})\hat{A}\delta(E'-\hat{H})\hat{B}\} \tag{3.7}$$

and

$$\rho(E) = e^{-\beta E}/Z \tag{3.8}$$

which yields for the correlation function

$$< \hat{A}(t)\hat{B}(t') >= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} J_{AB}(\omega). \tag{3.9}$$

Interchanging the order of the product and E and E′ yields

$$< \hat{B}(t')\hat{A}(t) >= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} e^{\beta\hbar\omega} J_{AB}(\omega) \tag{3.10}$$

since $\rho(E+\hbar\omega) = \rho(E)e^{-\beta\hbar\omega}$. This leads to a simple relationship between the ensemble average of the commutator and anticommutator of $\hat{A}$ and $\hat{B}$ which is referred to as the fluctuation-dissipation theorem[51, 54]. Unfortunately this factorization is not possible over the complete integration range if ρ in eq. (3.4) is replaced by $\rho_{q\neq 1}$. Hence, in principle, for $q \neq 1$ condensation may occur in dimensions $d \leq 3$.

We demonstrate, for interest sake, the following application of this result. Consider an ideal Bose gas for which the number of bosons is given by

$$N(\mu, T) = \int\int d^d r d^d p f_q(\epsilon) \tag{3.11}$$

$$\sim \int_0^{\infty} d\epsilon \epsilon^{\frac{d}{2}-1} f_q(\epsilon) \tag{3.12}$$

where d is the dimensionality and f_q is given by the Bose distribution

$$f_q = \frac{1}{[1+\beta(q-1)\epsilon_k]^{\frac{1}{q-1}} - 1}. \tag{3.13}$$

For q=1 it is easy to show that $\lim_{\mu\to 0} N_{q=1}(\mu, T)$ is divergent for d=1,2[55, 54] and condensation only occurs for d=3. On the other hand for q=2, $\lim_{\mu\to 0} N_{q=2}(\mu, T)$ is not convergent for d=1,2 or 3 which in spite of the absence of the fluctuation-dissipation theorem rules out the possibility of condensation.

In summary we conclude that it is acceptable to construct a 2D-BCS model of high-T_c superconductivity, provided we remain within the realm of generalized statistics, where the fluctuation-dissipation theorem is invalidated.

Chapter 4

BCS Theory and the Generalized Gap Equation

BCS theory is based on the assumption that, in a Fermi gas, normal state electrons near the Fermi surface may experience an effective attractive interaction due to polarization of the ionic lattice (electron-phonon-electron interaction). The Hamiltonian describing the energetics of electrons in such a system was postulated as follows

$$\hat{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\mathbf{k_1},\sigma_1,\mathbf{k_2},\sigma_2} c^{\dagger}_{\mathbf{k_1+s},\sigma_1} c^{\dagger}_{\mathbf{k_2-s},\sigma_2} g_{\mathbf{k_1},\mathbf{k_2},\mathbf{s}} c_{\mathbf{k_2},\sigma_2} c_{\mathbf{k_1},\sigma_1} \tag{4.1}$$

where $c^{\dagger}$ and c represent the usual Fermion creation and annihilation operators, corresponding to a state with momentum $\mathbf{k}$ and spin σ. The first term describes the kinetic energy and here $\varepsilon_{\mathbf{k}}$ stands for $\hbar^2 k^2/2m_e - \mu$, where again μ is the chemical potential. The second term represents the interaction between electrons quantified by the matrix element $g_{\mathbf{k_1},\mathbf{k_2},\mathbf{s}}$. It has the effect of taking a pair from a state $\mathbf{k_2}, \sigma_2; \mathbf{k_1}, \sigma_1$ and scattering it into a state $\mathbf{k_1} + \mathbf{s}, \sigma_1; \mathbf{k_2} - \mathbf{s}, \sigma_2$ so that both the scattered state and original state have the same total momentum. This might seem like a trivial statement. It is however the very foundation on which BCS theory is laid. It has the effect of creating a superfluid groundstate $|BCS\rangle$ consisting of pairs of electrons all having the same pair momentum.

Minimizing the corresponding free energy, one obtains at finite temperature the gap equation

$$\Delta_p = -\sum_k g_{kp}\frac{\Delta_k}{2E_k}(1 - f_{k\uparrow} - f_{k\downarrow}). \tag{4.2}$$

$f_{k\sigma}$ is the distribution function and E_k the quasi-particle energy given by

$$E_k^2 = \varepsilon_k^2 + \Delta^2 \tag{4.3}$$

with Δ the energy gap. In the BG case for weak coupling superconductors, the distribution function is the Fermi distribution and

$$\Delta_p = -\sum_k g_{kp}\frac{\Delta_k}{E_k}\tanh\frac{1}{2}\beta E_k. \tag{4.4}$$

Chosing at the outset S_q (2.3) for the entropy leads to f_q (2.14) in eq.(4.2) and changing the sum to an integral over the density of states, we obtain in 2D the generalized form of the gap equation:

$$\frac{1}{N(0)g} = \int \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2}}\frac{[1+\beta(q-1)\sqrt{\varepsilon^2+\Delta^2}]^{\frac{1}{q-1}} - 1}{[1+\beta(q-1)\sqrt{\varepsilon^2+\Delta^2}]^{\frac{1}{q-1}} + 1} \tag{4.5}$$

where $N(0)$ represents the density of states. For q=1 in 3D, one recovers the integral representation of(4.4) and, of course, a description of normal superconductors in the weak coupling limit. As required, equation (4.5) is independent of the distribution function at zero temperature where it reduces to

$$\frac{1}{N(0)g} = \int \frac{d\varepsilon}{(\Delta_0^2+\varepsilon^2)^{\frac{1}{2}}}. \tag{4.6}$$

Δ_0 being the zero temperature gap.

Let us, as a starting point, choose the usual BCS value as cutoff to the gap equation i.e. the Debye frequency $\hbar\omega_D$. Then the analytical solution to equation (4.6) is

$$\Delta_0 = (\hbar\omega_D + \sqrt{\hbar\omega_D^2 + \Delta_0^2})e^{\frac{-1}{N(0)g}}. \tag{4.7}$$

Using experimental values for the gap and Debye frequency, one can solve for $N(0)g$ at zero temperature. The problem reduces to finding that q in the gap equation, which yields a vanishing gap at the critical temperature and the same $N(0)g$. With q thus fixed, the temperature dependence of the gap can be determined.

It is at this stage appropriate to note that despite reasonable physical arguments in the case of normal superconductors, the choice of the Debye frequency as a cutoff is mathematically quite arbitrary. The temperature dependent solution to the gap equation in fact converges to a well defined value for any cutoff of sufficient magnitude. It is only when the cutoff is of a magnitude of the order of the gap itself, that deviations occur. In normal superconductors the Debye frequency is greater than the gap by $\sim 10^2$ and thus adequate. This is, however, certainly not the case in high-T_c superconductors where the gap at zero temperature may even be larger than the Debye frequency, e.g. in $Tl_2Ba_2Ca_2Cu_3O_{10}$ [56] (see [57] for Debye frequencies of other high T_c superconductors). Abandoning the Debye frequency as a cutoff is tantamount to acknowledging that the electron-phonon interaction is not the only interaction involved in forming of the condensed state.

It is interesting to note that the convergence of the gap at greater cutoffs, is accompanied by a simultaneous convergence of q. Consider a transformation of the gap in equation (4.5) via the substitution $\varepsilon = \frac{k_B T_c \varepsilon'}{2}$. Let us also define the cutoff in terms of multiples of the energy gap, *e.g.* $n\Delta_0$. Then for a given value of the gap to critical temperature ratio, $\frac{2\Delta_0}{k_B T_c} = m$, one can show that the gap equation reduces to a form dependent only on the ratio $\frac{2\Delta_0}{k_B T_c}$, the number n and q, and not on either the gap or critical temperature directly.

$$\frac{1}{N(0)g} = \int_0^{mn} \frac{d\varepsilon'}{\varepsilon'} \frac{[1+(q-1)\varepsilon'/2]^{\frac{1}{q-1}} - 1}{[1+(q-1)\varepsilon'/2]^{\frac{1}{q-1}} + 1} \tag{4.8}$$

Thus, if for a specific ratio of Δ_0 to T_c, the temperature dependent gap is convergent independent of cutoff, q must have a uniquely defined value. It therefore seems appropriate to define the cutoff in terms of the convergence of q, as this can be specified independently of the critical temperature pertaining to a specific material.

A relevant question now, is whether a generalization of the BCS universality condition of $\frac{2\Delta_0}{k_B T_c} \sim 3.52$ exists for the generalized statistics of Tsallis. Clearly the generalization must be q dependent because of the dependence of T_c on q and reduce to the BCS universality condition for q=1. In figure 4 a graph of $\frac{2\Delta_0}{q k_B T_c}$ versus q is given. This ratio does not deviate appreciably from 3.5 which suggests the following generalization

$$\frac{2\Delta_0}{q k_B T_c} \sim 3.52 \tag{4.9}$$

A more detailed analysis might lead to replacing q by some function of q which should be $\sim q$.

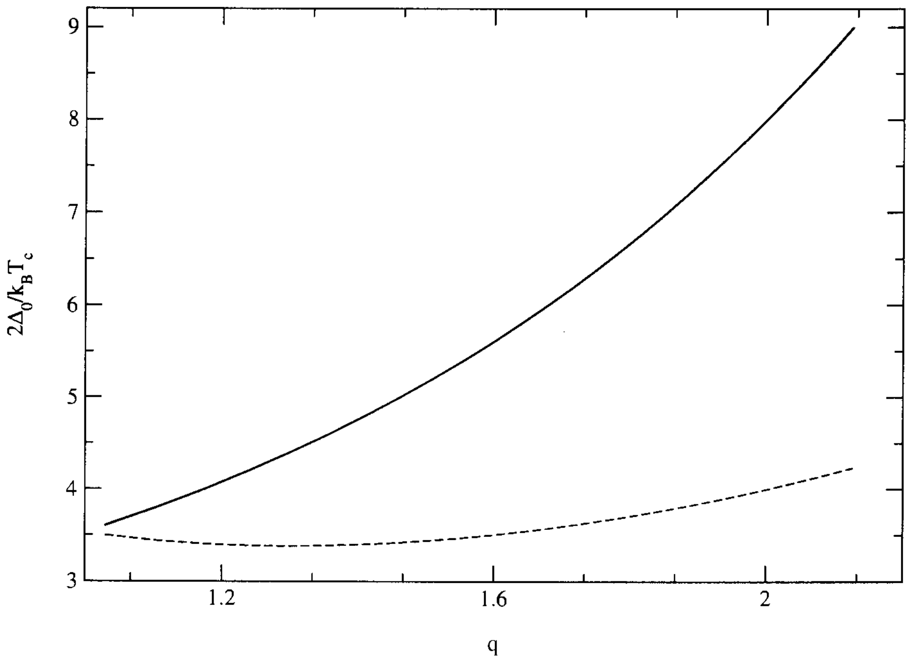

Figure 4.1: The ratio $\frac{2\Delta_0}{k_BT_c}$ vs. q is given by the solid curve. For comparison the dashed curve representing $\frac{2\Delta_0}{qk_BT_c}$ vs. q is included.

Chapter 5

Physical Properties

In this chapter we investigate some of the consequences of introducing generalized statistics into the BCS equations at finite temperature for measurable physical properties. Particular attention is paid to those properties mentioned in the introduction as characteristic of the cuprates.

5.1 The Isotope Effect

In BCS theory, the solution of the gap equation at T_c yields

$$kT_c = 1.14k\theta_D e^{\frac{-1}{N(0)g}}. \tag{5.1}$$

This linear dependence on θ_D predicts a corresponding dependence on the isotopic mass (M) of the phonon mediating ions: $T_c \sim \sqrt{\frac{1}{M}}$. The question now arises whether the incorporation of non-BG statistics will retain this dependence.

Consider the gap in equation (4.2) at T_c, independent of any particular choice of statistics and with the Debye frequency as choice of cutoff. A change in the integration variable $\varepsilon \rightarrow \epsilon k_B T_c$ may always be made such that the integration limits are from 0 to $\frac{\theta_D}{T_c}$. Integrating by parts yields:

$$\frac{1}{N(0)g} = [ln\epsilon(1-2f(\epsilon))]_0^{\frac{\theta_D}{T_c}} - \int_0^{\frac{\theta_D}{T_c}} (\epsilon - 2F(\epsilon)) \ln \epsilon \quad d\epsilon \tag{5.2}$$

where F(ϵ) is the indefinite integral of f(ϵ). In the first term on the right, the evaluation at zero must vanish, leaving:

$$\frac{1}{N(0)g} = (1-2f(\frac{\theta_D}{T_c}))\ln\frac{\theta_D}{T_c} - \int_0^{\frac{\theta_D}{T_c}} (\epsilon - 2F(\epsilon)) \ln \epsilon \quad d\epsilon \tag{5.3}$$

Taking the integral on the right to the left hand side and dividing by $(1-2f(\frac{\theta_D}{T_c}))$ yields some number φ which depends on the choice of $f(\epsilon)$. Exponentiating both sides yields:

$$T_c = \theta_D e^{\varphi} \tag{5.4}$$

which clearly demonstrates that the isotope effect is preserved in the BCS formulation irrespective of the particular form of statistical mechanics employed.

We have motivated the need to change the cutoff and this will, of course, influence this relation. It might be argued that the observed suppression in the isotope effect is a consequence of this.

5.2 Electronic Specific Heat

The electronic specific heat capacity may be expressed as

$$C = T\frac{dS}{dT} \tag{5.5}$$

where the entropy is given by

$$S_q = 2k_B[\frac{\int d\varepsilon\{f(E) - f(E)^q\}}{q-1} + \frac{\int d\varepsilon\{(1-f(E)) - (1-f(E))^q\}}{q-1}] \tag{5.6}$$

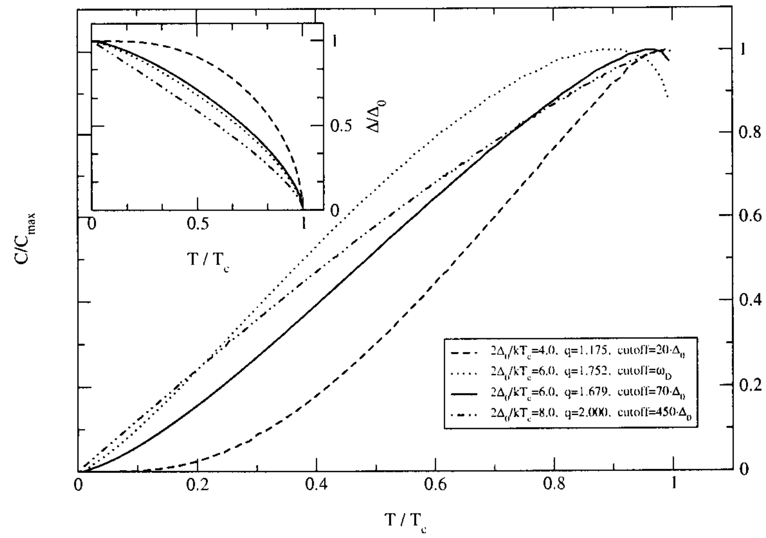

Figure 5.1: The normalized electronic specific heats $\frac{C}{C_{max}}$ vs. $\frac{T}{T_C}$ for various choices of $\frac{2\Delta_0}{k_B T_c}$, q and cutoffs where in each case C_{max} corresponds to the maximum value of C. The dotted line results from integrating to a cutoff of 390K which corresponds to the accepted value of the Debye temperature of LSCO. Corresponding values of the normalized gaps are shown in the inset.

and we use $N(0) = \frac{m}{2\pi\hbar^2}$ for the density of states in 2D and the bare electron mass m_e in all cases. 2D carrier densities given by Harshman and Mills [58] were used to convert the specific heat phase space integrals (2D) to amount of substance (mol) concentrations. The effect of the cutoff on the specific heat is shown in figure 5.2 for LSCO ($T_c = 36K$).

The linear nature of the specific heat can be seen over most of the superconducting region with $\hbar\omega_D = 390K$ as the cutoff. Clearly the situation deteriorates as the critical temperature is reached. Applying a linear regression to the 'most linear' part of C (between 0K and approximately $\frac{T}{T_c} = 0.65$) yields a slope of γ = 5.5 mJ/mol·K^2. Increasing the cutoff to $70\Delta_0$ yields a more linear form of the specific heat near T_c with little change in the shape of the gap (see inset in figure 5.2). Changing the cutoff from $\hbar\omega_D$ to $70\Delta_0$ increases the γ from to 10.7 mJ/mol·K^2 with a slight change in q (from 1.752 to 1.679). Note that in spite of the fact that the slopes of the specific heat may be altered by using an effective mass ($\gamma \rightarrow \frac{m_e^*}{m_e}\gamma$), these values are not in disagreement with many of the experimental results which seem to lie between 3 and 12 mJ/mol·K^2 for most cuprates [57]. For comparison the results for the specific heats and the gaps corresponding to ratios of $\frac{2\Delta_0}{k_B T_c} = 4.0$ and 8.0 are shown. Note the specific heat is much more linear when larger cutoffs are used and that the nonlinearity around T_c disappears almost completely for $\frac{2\Delta_0}{k_B T_c} = 8.0$, for which the slope increases to γ = 20.0 J/mol·K^2 and the cutoff = 450·Δ_0.

Little experimental data is available on the temperature dependence of the energy gap in cuprates. In figure 5.2 the experimental data obtained by Briceno and Zettl [4] for $Bi_2Sr_2CaCu_2O_8$ with $T_c = 85K$ and $\frac{2\Delta_0}{k_B T_c} = 6.2$ is compared with the theoretical results with q=1.717. In spite of a corresponding linear specific heat (γ = 13.9 mJ/mol·K^2 using m_e), the shape of the gap is not in exact agreement with their result.

5.3 Critical Field

Due to the type II nature of the cuprate oxides, a full analysis of the critical magnetic field would require including contributions to the free energy resulting from the flux lattice as well as the mutual energy of the surface current and flux line currents. We therefore present only a qualita-

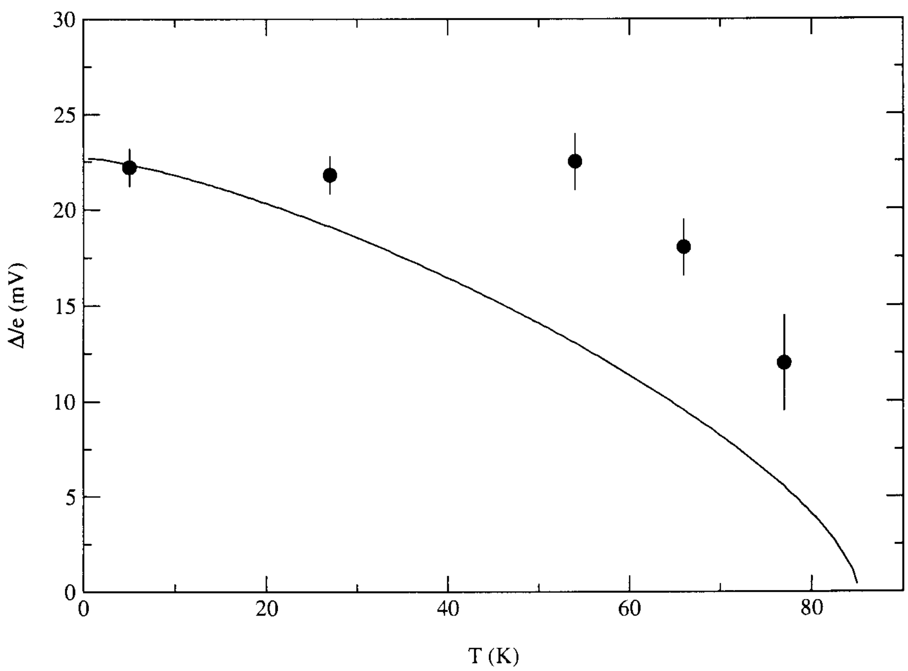

Figure 5.2: Comparison of the temperature dependence of experimental values of Δ from Ref [4] for $Bi_2Sr_2CaCu_2O_8$ with $T_c = 85K$ and $\frac{2\Delta_0}{k_B T_c} = 6.2$, with the theoretical results for q=1.71

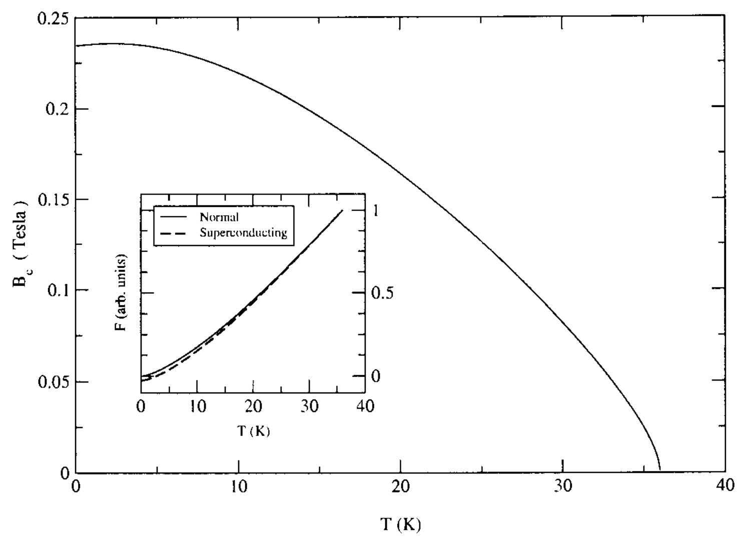

Figure 5.3: The critical magnetic field B_c vs. T obtained from free energies given in the inset.

tive analysis of the thermodynamic critical field, B_c, and make no attempt at solving either the lower- (B_{c1}) or upper- (B_{c2}) critical fields.

In 2D, the thermodynamic critical field is given by

$$\frac{B_c^2}{2\mu_0} = F_n - F_s \tag{5.7}$$

where F_n and F_s are the free energies in the normal- and superconducting states respectively, and μ_0 is the permeability of free space. The free energy can be written as

$$\begin{aligned} F &= 2\sum_k |\varepsilon_k|[f_k + (1-2f_k)h_k] \\ &- \sum_{k,k'} V_{k,k'}[h_k(1-h_k)h_{k'}(1-h_{k'})]^{\frac{1}{2}} \times \{(1-2f_k)(1-2f_{k'})\} - TS \end{aligned}$$

(5.8)

h_k is of the form

$$h_k = \frac{1}{2}[1 - \frac{\varepsilon_k}{E_k}]. \tag{5.9}$$

Upon substituting equation(2.14) and after some lengthy but straightforward algebra, our final result is

$$\begin{aligned} F_s &= N(0)(\hbar\omega)^2[[1 + (\frac{\Delta_0}{\hbar\omega})^2]^{\frac{1}{2}} - 1] - 2N(0)\int d\varepsilon(\frac{2\varepsilon^2 + \Delta^2}{E})f_q(\beta E) \\ &\quad - \frac{4kT}{q-1}N(0)\int d\varepsilon[(1 - f_q(\beta E))^q - (1 - f_q(\beta E))]. \end{aligned} \tag{5.10}$$

The question now arises whether the usual form for the normal state energy, $F_n = -\frac{1}{3}\pi^2 N(0)(k_B T)^2$, is still appropriate. Clearly, if $q \neq 1$ is used, F_s will not approach the normal state F_n as the gap vanishes at T_c, thus implying the existence of a non-zero critical field. This is of course experimentally unacceptable and demands that we postulate the normal state to also obey the generalized statistics.

Figure 5.3 shows the thermodynamic field obtained for a superconductor with $\frac{2\Delta_0}{k_B T_c} = 6.0$ and T_c = 36K . The inset shows the behaviour of the free energies. They differ from the weak coupled normal superconductor case where the free energy is always negative except at $T = 0$ at which point it vanishes. The difference, however, remains a positive definite quantity and no problems arise in calculating B_c. The zero temperature result of figure 5.3 agrees exceptionally well with an extrapolation based on experimental results due to [59]. They find, for a $La_{1.846}Sr_{0.154}CuO_4$ crystal with T_c = 35K that B_c = 0.251 T, while our results is 0.234 T.

5.4 The Josephson Effect

In this section we consider the effect of using generalized statistics on the current between two superconductors in contact via a tunneling barrier under an applied voltage. Effects resulting from the distinct tunneling mechanisms between superconductors are broadly referred to as Josephson effects[60]. Cohen *et al.* [61] first successfully described the tunneling of particles between superconductors. They considered a typical tunneling Hamiltonian of the form

$$H = H_L + H_R + H_T \tag{5.11}$$

where H_L and H_R are the complete Hamiltonians of the left and right sides of the tunneling barrier and H_T a tunneling term of the form

$$H_T = \sum_{L,R} T_{L,R}(c_L^\dagger c_R + c_R^\dagger c_L). \tag{5.12}$$

$T_{L,R}$ is the matrix element of the term, while $c_\alpha^\dagger$ and c_α are again the usual single particle creation and annihilation operators. The effect of this term is to take a particle from the one side of the barrier and transfer it to the other side. Josephson subsequently pointed out the need to take into account the tunneling not only of single particles, but also of pairs. This leads to a total tunneling current consisting of three contributions and dependent on the difference in phase, ϕ, of the superconducting states on the right and left sides

$$I(V,T) = I_{J1}(V,T)\sin\phi + I_{J2}\cos\phi + I_{qp}(V,T). \tag{5.13}$$

I_{qp} is the quasi-particle tunneling current, I_{J1} the coherent tunneling of pairs, while I_{J2} can be viewed as describing the tunneling of ordinary quasi-particles with a phase dependence. Integral expressions for all three terms were given by Ambegaokar and Baratoff [62], and also by Werthamer [63]. Larkin and Ovchinnikov [64] used an equivalent approach to simplify the expressions to single integrals, thus making the numerical analysis more tractable. We've used the expressions derived by the latter which are

$$\begin{aligned} I_{J1} &= \frac{\Delta_1\Delta_2}{2eR_N}\int_{-\infty}^{\infty}\Big(\frac{\theta(\Delta_1-|\omega-eV|)\theta(|\omega|-\Delta_2)}{(\Delta_1^2-(\omega-eV)^2)^{\frac{1}{2}}[\omega^2-\Delta_2^2]^{\frac{1}{2}}} \\ &\quad+\frac{\theta(|\omega|-\Delta_1)\theta(\Delta_2-|\omega+eV|)}{(\omega^2-\Delta_1^2)^{\frac{1}{2}}[\Delta_2^2-(\omega+eV)^2]^{\frac{1}{2}}}\Big)\times[1-2f(|\omega|)]d\omega \end{aligned} \tag{5.14}$$

$$\begin{aligned} I_{J2} &= -\frac{\Delta_1\Delta_2}{eR_N}\int_{-\infty}^{\infty}\frac{(sgn\omega)[sgn(\omega+eV)]\theta(|\omega|-\Delta_1)\theta(|\omega+eV|-\Delta_2)}{(\omega^2-\Delta_1^2)^{\frac{1}{2}}[(\omega+eV)^2-\Delta_2^2]^{\frac{1}{2}}} \\ &\quad\times[f(\omega+eV)-f(\omega)]d\omega \end{aligned} \tag{5.15}$$

and

$$\begin{aligned} I_{qp} &= \frac{1}{eR_N}\int_{-\infty}^{\infty}\frac{|\omega||\omega+eV|\theta(|\omega|-\Delta_1)\theta(|\omega+eV|-\Delta_2)}{(\omega^2-\Delta_1^2)^{\frac{1}{2}}[(\omega+eV)^2-\Delta_2^2]^{\frac{1}{2}}} \\ &\quad\times[f(\omega)-f(\omega+eV)]d\omega \end{aligned} \tag{5.16}$$

where

$$\begin{aligned} sgn(\omega) &= +1 \quad for \quad \omega>0 \\ &= -1 \quad for \quad \omega<0, \\ \theta(\omega) &= 0 \quad for \quad \omega<0 \\ &= 1 \quad for \quad \omega>0 \end{aligned} \tag{5.17}$$

and V is the applied voltage, e the electron charge, R_N the junction resistance and Δ_1, Δ_2 the energy gap on either side of the tunneling junction. A summary of much of the fundamental work is given by Harris [65].

Equations (5.14)-(5.16) apply to 3D where the junction resistance is expressed in terms of the microscopic quantities [66]: the density of states at the Fermi level, the matrix element and fundamental constants. This we assume to be a macroscopicly measurable quantity and no problems arise in directly using (5.14)-(5.16) in the 2D case, if results are expressed as $I \cdot R_N$.

The main difficulty in evaluating the tunneling currents is the presence of square root singularities, due to the denominator becoming zero for certain values of the integration variable ω in (5.14)- (5.16). The appropriate method to deal with these singularities was demonstrated by Shapiro *et al.* [67]. A detailed discussion of his approach is given in Appendix A. One frequently applied, and apparently indispensable step in this approach, is a transformation of the variable of integration $\omega \rightarrow -\omega$, see equation (A.12). This leads to another complication. The generalized distribution function contains terms of the form

$$[1 + \beta(q-1)\epsilon]^{\frac{1}{q-1}}. \tag{5.18}$$

The change in sign of ω might lead, in this case, to a negative value of the argument ϵ and consequently a negative under the power $\frac{1}{q-1}$. This seems to be an inherent difficulty of the Tsallis formulation, which requires a cutoff to the integration boundaries whenever (5.18) becomes imaginary. We propose, however, that a perfectly valid, and in some respects a more consistent, generalization of BG statistics can be made by writing any term e^{-x} in the BG case as

$$e^{-x} \quad \rightarrow \quad \frac{1}{e^x} \tag{5.19}$$

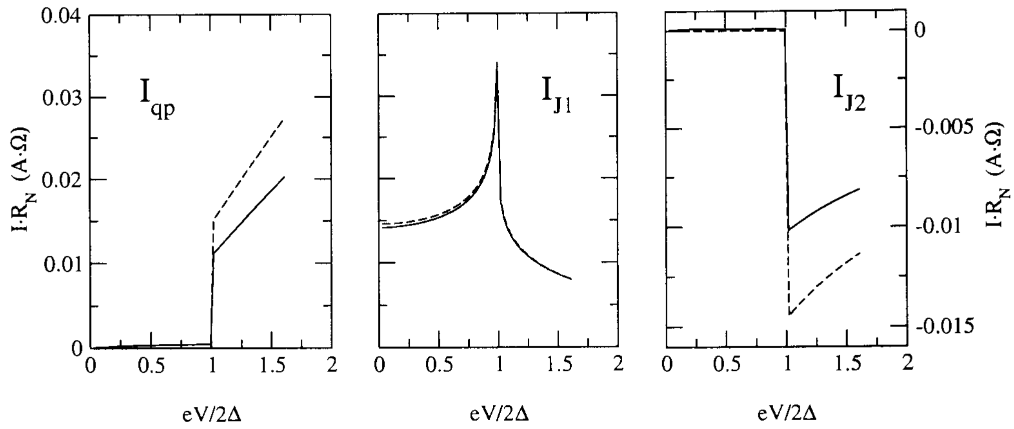

Figure 5.4: Various components of the total tunneling current for a tunnel junction between two identical superconductors at 5K with an energy gap of $\frac{2\Delta}{k_B T_c} = 6.0$. Dashed lines indicate BG calculations while solid lines show the generalized results with $q = 1.679$.

and analogously in the generalized case

$$[1 + \beta(q-1)(-|\epsilon|)]^{\frac{1}{q-1}} \quad \rightarrow \quad \frac{1}{[1 + \beta(q-1)|\epsilon|]^{\frac{1}{q-1}}} \tag{5.20}$$

In both formulations the BG exponential is retrieved as $q \rightarrow 1$ and both are therefore equally valid. No complication arises due to an imaginary term in the latter and the integration may be done over the whole region. This was used whenever applicable.

In Figure 5.4 we show the result of evaluating equations (5.14)-(5.16) at 5K for a junction with identical superconductors with $\frac{2\Delta_0}{k_B T_c} = 6.0$ and using the generalized distribution function with q=1.679. The results are compared to the equivalent calculation using BG statistics to illustrate the

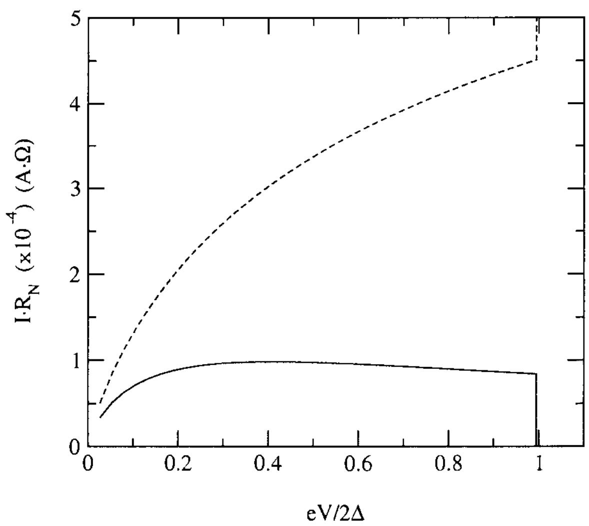

Figure 5.5: Generalized I_{J2}(solid line) and I_{qp}(dashed line) in the region $eV < 2\Delta$. Note that a BG calculation yields a negligible contribution in this region.

effect of the choice of statistics. Of interest is significant contributions of I_{J2} and I_{qp} below an applied voltage of $2\Delta/e$. The BG calculation yields a negligible contribution in this region at low temperatures. In figure 5.5 the $eV < 2\Delta$ region is magnified for clarity.

One feature that has emerged experimentally, is the presence of a peak in the conductance spectrum $\frac{dI}{dV}$ of certain high-T_c's at zero bias and low temperatures [68, 9] . No peak of this nature can arise in the BG case, as both I_{qp} and I_{J2} are effectively negligible and the derivative of I_{J1} is zero at $V = 0$. The existence of finite contributions are, however, clearly illustrated in figures 5.4 and 5.5 for the generalized case. Although the precise structure observed experimentally is not seen here, the existence of these contributions raises the possibility that interference due to other admixtures, perhaps d-wave or Andreev bound states, will produce the sought after structure.

The use of generalized statistics in the BCS equations thus allows the experimentally observed discontinuities in the tunneling currents to be interpreted as being coincident with the energy gap at low T, whilst consistently predicting the gap to vanish at the correct critical temperature.

5.5 Discussion

We have thus far shown that many of the characteristic properties of the high-T_c's may be predicted by generalization of the distribution function. A couple of general comments are in order.

An obvious question that might arise regards the conclusion that the generalized distribution function need also apply to the normal state. Certainly the normal state of cuprates does not display surprising or anomalous properties that might lead one to postulate the need for a generalization of the entropic measure. One would want to verify that these properties can indeed appear within the generalized formulation, without appreciable deviation from the expected behaviour within BG statistics. To this end we compare the normal state entropy, $S(T)$, in the BG case with the generalized case for an arbitrarily chosen q, figure 5.6. In the BG case one expects to see a linear entropy as illustrated (which through $T\frac{dS}{dT}$ leads to a linear specific heat). In figure 5.6 the result of increasing the integration cutoff in the generalized entropy is shown. This removes the non linear behaviour in the entropy. As a larger cutoff was also required in the superconducting state, this is consistent with the proposed scheme. Clearly the order of magnitude of the BG prediction is different, but nothing anoma-

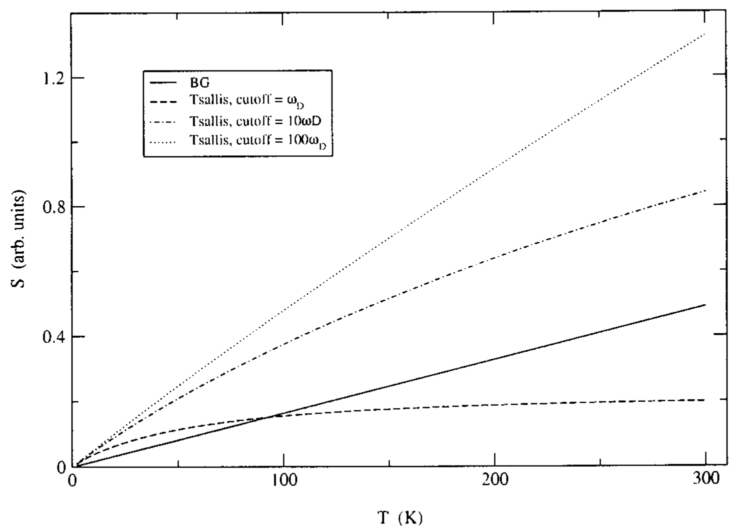

Figure 5.6: Comparison of the BG entropy in the normal state to the generalized case for various cutoffs. An arbitrary Debye frequency, $\omega_D = 390K$, and $q = 1.679$ were chosen. Note the generalized entropy becomes more linear with increased cutoff.

lous occurs.

Finally, a point to ponder is a possible prediction for the limit that T_c might attain. This is presumably critically linked to the physical interpretation of the value q. One might argue that high-T_c superconductivity results from a particular type of dynamics and that it pertains to a very specific value of q or at worst a very small range of q's. This conveniently fixes another applicable parameter. In our proposed universality condition (4.9) one can always substitute the analytical solution (4.7) for the zero temperature energy gap Δ_0. A relation is then obtained between q, T_c and the coupling strength which may very well too be q-dependent. Ultimately this is the relevant relation as it links T_c to that physical effect responsible for the existence of the superconducting state, i.e. the coupling. It appears as though no definite answer will emerge until a better understanding of the nature of q and the material properties of the cuprates that lead to the non-extensive dynamics is uncovered.

In conclusion a simple 2D s-wave BCS pairing model which incorporates generalized statistics has been proposed as a mechanism leading to high critical temperatures in the cuprate family of superconductors. A physical interpretation fixing energy cutoffs of the divergent phase space integrals is still lacking in this formalism. Nonetheless an adequate description of many of the main features can be achieved, if non-phonon mediated interactions are assumed to extend the excitation spectrum beyond the Debye frequency.

Appendix A

Josephson Integrals

The square root singularities in the Josephson integrals were first treated by Shapiro *et al.* [67]. A detailed analysis of his approach for a junction with identical superconductors is given. Consider the quasiparticle current in equation (5.16), but with the denominator factorized:

$$I_{qp} = \frac{1}{eR_N}\int_{-\infty}^{\infty}\frac{|\omega||\omega+eV|\theta(|\omega|-\Delta)\theta(|\omega+eV|-\Delta)}{\sqrt{(\omega-\Delta)(\omega+\Delta)(\omega+eV-\Delta)(\omega+eV+\Delta)}} \times[f(\omega)-f(\omega+eV)]d\omega \quad \text{(A.1)}$$

The crux of the approach is to make a transformation of the variable of integration such that terms under the square root that might cause singularities are canceled out. The θ step functions in the numerator define different integration regions in which the integrand is non-zero, depending on the magnitude of V. The integral must be solved independently in each region. From (A.1)

$$|\omega| > \Delta$$
$$|\omega + eV| > \Delta.$$

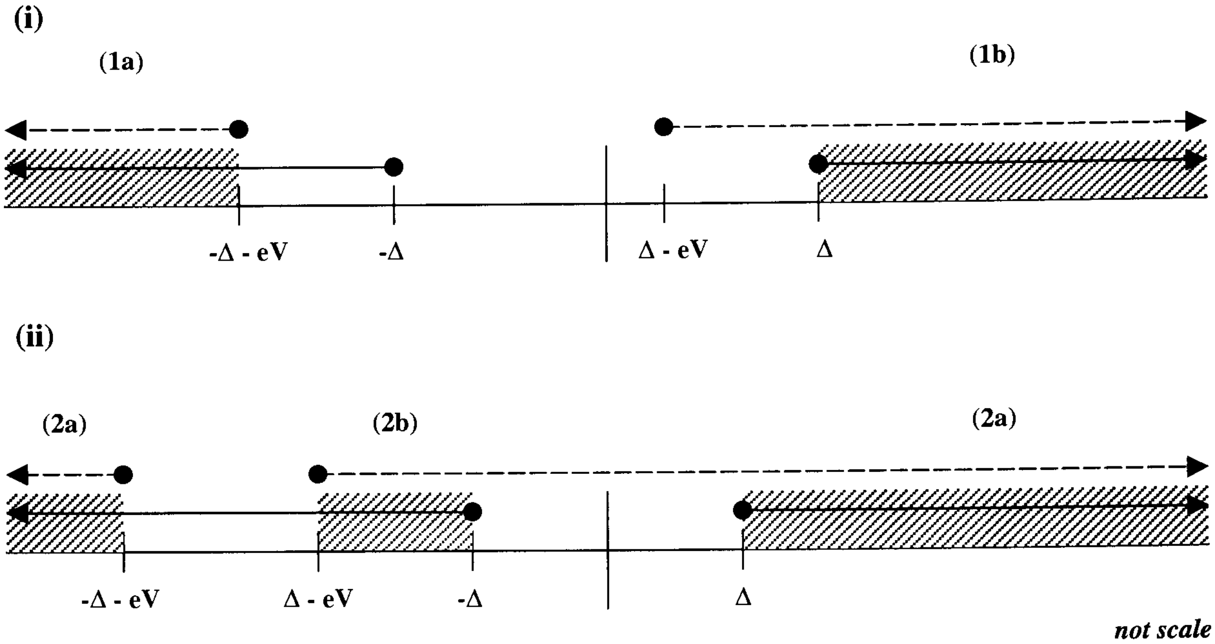

Figure A.1: Graphical representation of the integration regions defined by the θ-step functions in equation (A.1). The top number line applies to the applied voltages of magnitude $0 < eV < 2\Delta$, while the bottom is for voltages $eV > 2\Delta$. The shaded areas indicate regions where the two θ-functions are simultaneously non-zero and hence where the integral should be solved.

Graphically this can be visualized as shown in figure A.

Consider first the situation in figure A(i) i.e. $eV < 2\Delta$. The current must be solved independently in the two integration regions, indicated by the two shaded areas (1a) and (1b).

Define current I_{1a} as the current in region (1a), then

$$I_{1a} = \frac{1}{eR_N}\int_{-\infty}^{-\Delta-eV} \frac{|\omega||\omega+eV|}{\sqrt{(\omega-\Delta)(\omega+\Delta)(\omega+eV-\Delta)(\omega+eV+\Delta)}} \times[f(\omega)-f(\omega+eV)]d\omega. \tag{A.2}$$

The upper boundary causes singular behaviour due to the last term under the root. Now let

$$\left(\frac{\omega-\beta}{\alpha}\right)^2 = \cosh^2 u. \tag{A.3}$$

The singularity is canceled upon substitution, by defining

$$(\omega+eV-\Delta)(\omega+eV+\Delta) = \alpha^2\sinh^2 u. \tag{A.4}$$

The first term in brackets on the left in (A.4) may be chosen arbitrarily. α and β are consequently fixed and may be uniquely determined at the upper boundary $u = 0$. Here, from (A.3)

$$\omega = \beta \pm \alpha \tag{A.5}$$

and (A.4) becomes

$$(\omega+eV-\Delta)(\omega+eV+\Delta) = 0. \tag{A.6}$$

The last is true for two different values of ω (see (A.5))

$$\begin{aligned} \beta+\alpha &= -\Delta-eV \\ \beta-\alpha &= \Delta-eV \end{aligned} \tag{A.7}$$

From this it follows that

$$\begin{aligned} \alpha &= -\Delta \\ \beta &= -eV. \end{aligned} \tag{A.8}$$

which yields the final desired result

$$I_{1a} = \frac{1}{eR_N}\int_{-\infty}^{0} \frac{|\omega||\omega + eV|}{\sqrt{(\omega-\Delta)(\omega+\Delta)}} \times [f(\omega) - f(\omega+eV)]du \tag{A.9}$$

with

$$\omega = -\Delta \cosh u - eV. \tag{A.10}$$

(A.10) is the appropriate transformation of ω as $\omega = -\alpha \cosh u + \beta$ from (A.3) leads to a negative value under the root in (A.9). Equation (A.9) may be integrated numerically.

In the region (2b) in figure A, a somewhat different approach is required. In this case both integration limits are finite and therefore the cosh function is inappropriate. Here

$$I_{2b} = \frac{1}{eR_N}\int_{\Delta-eV}^{-\Delta} \frac{|\omega||\omega+eV|}{\sqrt{(\omega-\Delta)(\omega+\Delta)(\omega+eV-\Delta)(\omega+eV+\Delta)}}$$

$$\times[f(\omega) - f(\omega+eV)]d\omega \tag{A.11}$$

The second and third terms in brackets under the root cause singular behaviour at the upper and lower boundaries respectively, while the first term introduces a negative under the root. As only two terms can be canceled out in the current approach, it is necessary to first transform using $\omega \to -\omega$. Then

$$I_{2b} = \frac{1}{eR_N}\int_{\Delta}^{eV-\Delta} \frac{|-\omega||eV-\omega|}{\sqrt{(\omega-\Delta)(\omega+\Delta)(eV-\omega-\Delta)(eV-\omega+\Delta)}}$$

$$\times[f(-\omega) - f(eV-\omega)]d\omega \tag{A.12}$$

in which the first and third terms in brackets under the root become zero at the lower and upper boundaries respectively. Let

$$\left(\frac{\omega-\beta}{\alpha}\right)^2=\sin^2 u \tag{A.13}$$

and

$$(\omega-\Delta)(eV-\omega-\Delta)=\alpha^2\cos^2 u. \tag{A.14}$$

α and β are solved for at the boundaries $u=-\frac{\pi}{2}$ and $u=\frac{\pi}{2}$. The final result is

$$I_{2b}=\frac{1}{eR_N}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{|-\omega||eV-\omega|}{\sqrt{(\omega+\Delta)(eV-\omega+\Delta)}}\times[f(-\omega)-f(eV-\omega)]du \tag{A.15}$$

where

$$\omega=(\frac{eV}{2}-\Delta)\sin u+\frac{eV}{2}. \tag{A.16}$$

All Josephson integrals can be solved in a manner analogous to the methods described above. For a specific voltage the total current is just the sum of the solutions in each integration region.

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