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Bose–Einstein condensation in finite-length channels composed of weakly interacting filaments

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Abstract

Bose–Einstein condensation temperatures T_B for non-interacting bosons in square arrays of finite-length filaments arranged on a square lattice are calculated both by numerical methods and by use of a simple approximate theory which is appropriate in certain parameter ranges. It is assumed that both longitudinal and transverse motion can be described by constant effective masses M_L and M_T, but maximum wave vectors are introduced related to the filament lattice constant or to the filament separation. For large numbers of filaments a gradual crossover from $T_B \propto (1/M_L M_T)^{1/2}$ to $T_B \propto (1/M_L M_T^2)^{1/3}$ is found as parameters are varied to make $k_B T_B$ change from being larger than to smaller than the maximum transverse boson energy, W_T. For $k_B T_B > W_T$ it is shown that, in the absence of disorder, the number of filaments required to bring T_B up to a given fraction of its value for large numbers of filaments is approximately proportional to the filament lengths and to $(M_L/M_T)^{1/2}$. It is argued that disorder will act to flatten off any length dependence of this number above some length dependent on the amount of disorder. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

There is no Bose–Einstein condensation of non-interacting bosons with a quadratic dispersion relation in a one-dimensional system in the limit of infinite lengths [1]. However, as will be verified by calculations in this paper, condensation in the weak sense [2] of a temperature below which the occupation number of the ground state starts to become macroscopic, i.e., of the same order as the number of bosons, can occur in a finite-length one-dimensional system because of finite separations between successive energy levels, particularly between the states with the lowest and next-lowest energies.

In this paper we use the word filament to denote a quasi one-dimensional region in which current carriers can move along the region's length in a one-dimensional band, but are in the lowest-energy quantum state for transverse motion at all temperatures of interest. If pairs of electrons in such a filament are strongly bound, then a first approximate way to treat such a system could be to regard it as an ideal Bose gas in one dimension, although any interaction between pairs may have more serious consequences than in bulk material. This is certainly the case for fermions in one-dimensional systems [3].

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The main calculations of this paper are concerned with the problem of what happens in a square array of finite-length filaments on a simple square lattice, with the effect of overlaps of wave functions of different filaments approximated by inclusion of a transverse boson mass. Wave vectors in the longitudinal and transverse directions are assumed to be limited by (π/a_L) and (π/a_T), where a_L is the lattice constant in the direction of the filament length, and a_T is the separation between nearest-neighbour filaments. A particular case where longitudinal and transverse masses are equal and a_L and a_T tend to zero is equivalent to the problem of bosons in a rectangular box with infinite wall heights studied previously by other authors [4].

First we present numerical results for the condensation temperature T_B as a function of numbers of filaments for a few representative cases. These cases cover a range of ratios of longitudinal to transverse masses between 10^{-1} and 10^{-3}. Transverse boson masses can be expected to be fairly heavy if adjacent filaments are not too close.

After presentation of the numerical results, we show how these may be obtained approximately in some parameter ranges by analytical calculations which approximate the Bose–Einstein occupation factor by a term inversely proportional to the difference in energy between those excited states which play a significant part in the problem and the ground state, and then approximate sums over longitudinal wave vectors by integrals except for the case of the states with lowest energy with respect to transverse motion.

The work presented here could be applicable to arrays of quantum wires of doped semiconductors if they become superconducting. If so, then at low carrier concentrations, a Bose-gas model may be appropriate. Superconducting transition temperatures as high as about 50 K for plasmon-induced pairing have been predicted for quantum wells in CdS at an optimum carrier concentration [5].

Another semiconductor of interest in this connection is $SrTiO_3$, since it is superconducting at lower carrier concentrations than other known superconducting semiconductors. In $SrTiO_3$ with 3% of Ti replaced by Zr, there are strong indications that superconductivity on the Bose-gas side of the BCS–Bose gas transition has been seen in one ceramic sample with a very low carrier concentration [6–8] of the order of 10^{15} cm^{-3}. This observation gave qualitative confirmation of predictions made many years earlier for this material, although the pairing temperature inferred from experiments is about twenty times smaller than was predicted with the model used before [9].

The most promising way to make suitably oriented arrays of conducting filaments would be to use very narrow ion beams travelling parallel to a [111] direction of a thin $SrTiO_3$ sample. Ion beams which can be focused on areas with dimensions as small as 8 nm with a half angle of 0.15 mrad were reported several years ago [10]. Even for such a small beam angle it would probably be necessary to work with films in order to get filaments with a fairly uniform diameter. For a filament of diameter 8 nm, the largest carrier concentration which will permit all carriers to be in the lowest quantum state with respect to transverse motion can be calculated [11], for a three-valley model for the conduction band, to be 2×10^{19} cm^{-3}, implying a linear concentration per filament of about 1.3×10^{7} cm^{-1}. Probably, considerably lower carrier concentrations would be needed for the ratio of pair diameters in the filaments to the pair separation to become smaller than unity so that the Bose-gas regime could be approached.

Another use of the results presented here may be connected with assessment of the validity of a high-drift-velocity model developed by the present author [12–15] to give a possible explanation of claims of room-temperature superconductivity in narrow channels through films of oxidised atactic polypropylene [16–21] and polydimethylsiloxane [21]. It is expected that further discussion of this topic will be presented in a later paper.

Some numerical results for square arrays of filaments are shown in Section 2, and a simplified approximate theory for some ranges of parameters of interest is presented in Section 3. Conjectures about effects of disorder are made in Section 4.

2. Basic equations and numerical calculations for square arrays

We consider non-interacting bosons on a square array of filaments of length L on a simple square lattice, with the sides of the square of length D. We measure the length L and the transverse dimension D from points half a lattice constant a_L beyond the end lattice points of a filament, and half the nearest-neighbour interfilament distance a_T beyond the outermost filament rows. We suppose that the bosons have masses M_L and M_T in the filament direction and perpendicular to this, and call these longitudinal and transverse masses. We assume boundary conditions such that the boson wave functions vanish at the ends of the filaments and at the sides of the square. The boson states can be characterised by integers i,j,k, where i,j run from 1 to n_T, with $n_T = D/a_T$, and k runs from 1 to n_L, with $n_L = L/a_L$. The wave functions are proportional to $u_T(x)u_T(y)u_L(z)\sin(i\pi x/D)\sin(j\pi y/D)\sin(k\pi z/D)$, where u_T and u_L are periodic functions with periods a_T and a_L. The energy $E_B(i,j,k)$ of the state (i,j,k) measured from the lowest energy state (1,1,1) is given by

$$E_B(i,j,k) = E_T(i^2 + j^2 - 2) + E_L(k^2 - 1), \qquad (1)$$

where

$$\begin{aligned} E_T &= (\hbar^2/2M_T)(\pi/D)^2, \\ E_L &= (\hbar^2/2M_L)(\pi/L)^2. \end{aligned} \qquad (2)$$

Condensation into the lowest-energy state cannot take place if the sum of the boson occupation factors over all states except the lowest for a chemical potential situated at the energy of the lowest state is greater than the total number of bosons, N_B. Below the temperature at which this sum is equal to N_B, the occupation of the ground state will start to become macroscopic, i.e., of the order of N_B, and so the equality of the sum with N_B determines the condensation temperature T_B in this weak sense [2]. For an average linear concentration c of bosons per filament, this criterion can be written as

$$\sum_{i,j=1}^{n_T} \sum_{k=k_0}^{n_L} \frac{1}{\exp[E_B(i,j,k)/k_B T_B] - 1} = cLn_T^2, \qquad (3)$$

where $k_0 = 2$ if $i = j = 1$ and $k_0 = 1$ otherwise, and

$$n_T = D/a_T, \quad n_L = L/a_L \qquad (4)$$

are the numbers of different wave numbers in the transverse and longitudinal directions, respectively.

We have written a computer programme to calculate the ratio $(k_B T_B/E_L cL)$ with input required being values of: (i) cL, the average number of bosons per filament; (ii) the ratio r given by

$$r = (\hbar^2/2M_T a_T^2)/(\hbar^2/2M_L L^2), \qquad (5)$$

representing the ratio of the maximum transverse energy to the small characteristic longitudinal energy E_L depending on the filament length; (iii) n_T, the number of filaments in each row of the array; and (iv) n_L, the number of lattice constants per filament. The results are insensitive to n_L provided that it is large.

In Figs. 1–3, we plot the ratio $(k_B T_B/E_L cL)$ as a function of n_T on a log–log scale for $cL = 2000$, $(L/a_T) = 1000$, $n_L = 4000$, and values of (M_T/M_L) varying from 10^3 to 10.

For values of cL and n_L used for the numerical work for Figs. 1–3, the condensation temperature for a single filament satisfies $k_B T_B \approx 1.38\ E_L cL$, with E_L given by Eq. (2), and it is found that, for maximum transverse boson energies small compared with $k_B T_B$, the enhancement factor for large arrays is approximately $0.3r^{1/2}$. The single-filament condensation temperature is proportional to $(c/M_L L)$, and the enhancement factor for large arrays is approximately proportional to $[(M_L/M_T)^{1/2}(L/a_T)]$.

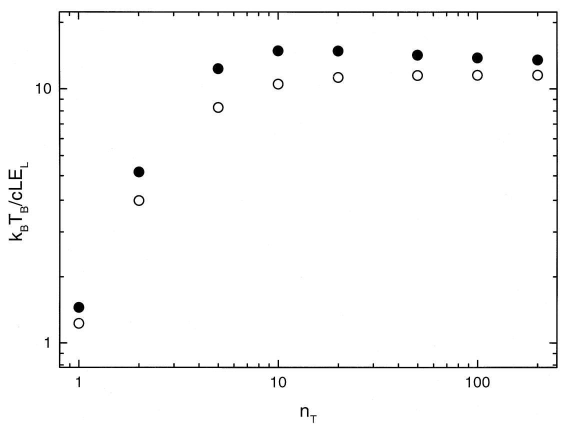

Fig. 1. Ratio $(k_B T_B/cLE_L)$ plotted against n_T for $(M_T/M_L) = 10^3$, $cL = 2000$, $(L/a_T) = 1000$ and $n_L = 4000$. Solid circles—numerical results from Eq. (3). Open circles—approximate results from Eq. (21).

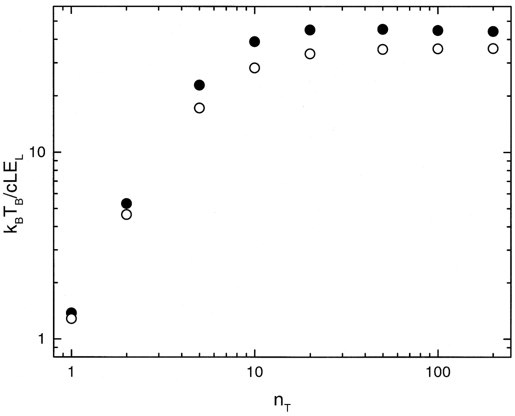

Fig. 2. As for Fig. 1, but with $(M_T/M_L) = 10^2$.

Under the same condition that the maximum transverse boson energy is small compared with $k_B T_B$, and if also E_T and E_L of Eq. (2) satisfy $E_T > E_L$, the characteristic number of filaments n_T^2 at which T_B reaches half its value for large n_T is also approximately equal to $0.3 r^{1/2}$. As an example, if $L = 2$ μm, $cL = 2000$, $M_L = m_e$, $M_T = 100 m_e$, $a_T = 2$ nm (giving $r = 10^4$), and $n_L = 4000$, we find that the single-filament $T_B = 3.0$ K, the enhancement factor at large n_T is about $32 (= 0.32 r^{1/2})$, and the value of n_T at which the enhancement is about half this value is such that $n_T^2 \approx 25 = 0.25 r^{1/2}$.

In Section 3, an approximate theory will be given which gives fair agreement with the numerical results in some parameter ranges. This approximate theory gives more insight into why the above statements about enhancement factors and their dependence on n_T are valid.

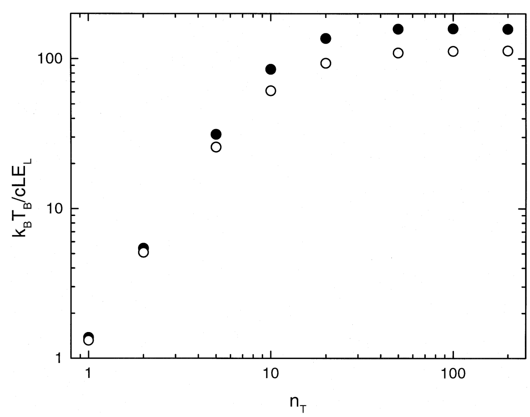

Fig. 3. As for Fig. 1, but with $(M_T/M_L) = 10$.

3. An approximate theory for small maximum transverse energies

For energies E_B smaller than about $0.5 k_B T_B$ it is a fair first approximation to replace the Bose–Einstein occupation number in Eq. (3) by

$$\frac{1}{\exp(E_B/k_B T_B) - 1} \approx (k_B T_B/E_B), \tag{6}$$

and we shall find empirically by comparison with numerical results that in many circumstances consideration of only those states for which this inverse linear approximation can be used in the sum of Eq. (3) gives a fair approximation to the sum.

For a given dimensionless transverse quantum number p_T defined by

$$p_T = \left(i^2 + j^2\right)^{1/2}, \tag{7}$$

we take the sum over k up to $k_m(p_T)$, where

$$k_m = \min\left(n_L, k_p\right), \tag{8}$$

with k_p given by

$$E_T\left(p_T^2 - 2\right) + E_L\left(k_p^2 - 1\right) = b k_B T_B, \tag{9}$$

where $b \sim 0.5$. If $p_T = 2^{1/2}$, then the sum can be performed exactly. We find the sum, $S(2^{1/2})$ is given by

$$S(2^{1/2}) = \frac{k_B T_B}{E_L} \sum_{k=2}^{k_m(2^{1/2})} \frac{1}{k^2 - 1} = \frac{k_B T_B}{2 E_L}\left(\frac{3}{2} - \frac{1}{k_m} - \frac{1}{k_m + 1}\right) \approx \frac{3}{4}\frac{k_B T_B}{E_L} \tag{10}$$

if $k_m(2^{1/2})$ is large. Hence, from Eq. (3), we see that $k_B T_B$ for the case of one filament is given by

$$k_B T_B \approx (4/3) E_L cL. \tag{11}$$

If $p_T > 2^{1/2}$, then the sum $S(p_T)$ for a given p_T is given by

$$S(p_T) = \frac{k_B T_B}{E_L} \sum_{k=1}^{k_m(p_T)} \frac{1}{k^2 - 1 + s\left(p_T^2 - 2\right)}, \tag{12}$$

where

$$s = E_T/E_L = r/n_T^2, \tag{13}$$

and r is defined by Eq. (5).

If $s > 1/3$, as is probable for $L \gg D$, then

$$S(p_T) = \frac{k_B T_B}{E_L} \sum_{k=1}^{k_m(p_T)} \frac{1}{k^2+q^2}, \tag{14}$$

where

$$q = \left[s\left(p_T^2-2\right)-1\right]^{1/2} \tag{15}$$

is real. If we approximate the sum by an integral from 0.5 to $[k_m(p_T)+0.5]$, we find

$$S(p_T) \approx \frac{k_B T_B}{E_L}\left[(1/q)\arctan(x/q)\right]_{0.5}^{k_m(p_T)+0.5}$$
$$\approx \frac{1}{q}\frac{k_B T_B}{E_L}\left[\frac{\pi}{2} - \arctan\left(\frac{1}{2q}\right)\right] \tag{16}$$

if k_m is large. This further reduces to

$$S(p_T) \approx \frac{1}{q}\frac{k_B T_B}{E_L}\frac{\pi}{2} \tag{17}$$

if q is large.

The integer $k_m(p_T)$ will be large if $n_L \gg 1$ and if

$$E_T\left(p_T^2-2\right) < \left[b - n^2(E_L/k_B T_B)\right] k_B T_B, \tag{18}$$

with $b \sim 0.5$ [see Eq. (9)] and n is some large number. If this inequality is satisfied for the maximum $p_T(=2^{1/2}n_T)$, and if $n_L \gg 1$ and $s \gg 1$, then the approximation of Eq. (16) can be used for all p_T except for $p_T = 2^{1/2}$ for which we can use the right-hand approximation of Eq. (10). We shall also make the further approximation that q of Eq. (15) is large for most values of p_T, and hence use Eq. (17) for $p_T \neq 2^{1/2}$. Hence, we find

$$cL \approx \frac{k_B T_B}{E_L}\left\{\frac{3}{4n_T^2} + \frac{\pi}{2s^{1/2}}\left(1-1/n_T^2\right)\mathrm{av}_{(i^2+j^2>2)}\left[\frac{1}{\left(i^2+j^2-2\right)^{1/2}}\right]\right\}. \tag{19}$$

For values of n_T which are greater than about 10 it is a fair approximation to ignore the 2 in (i^2+j^2-2) and replace the average in Eq. (19) by an integral average of $(1/\rho)$ over a square with sides of length $(n_T+0.5)$ with a small square with sides of length 0.5 removed from one corner, where ρ is the distance from that corner. With these approximations we find

$$\mathrm{av}\left[\frac{1}{\left(i^2+j^2-2\right)^{1/2}}\right] \approx (\pi/2n_T)/\{\ln[\tan(3\pi/8)]\}$$
$$= 1.782/n_T. \tag{20}$$

From Eqs. (19) and (20), after ignoring the term $(1/n_T^2)$ in $(1-1/n_T^2)$ in Eq. (19), we deduce that

$$k_B T_B \approx (4/3)(cLE_L)\left[\frac{1}{\left(1/n_T^2 + 3.73/r^{1/2}\right)}\right], \tag{21}$$

with r given by Eq. (5). Since the second term in the denominator of Eq. (21) is only correct to first order in $(1/n_T)$, the equation will be a poor approximation for small n_T unless $r^{1/2}(=n_T s^{1/2})$ is large. For $n_T = 1$ the earlier expression of Eq. (11) is more appropriate to use.

We see from Eq. (21) that the maximum enhancement factor of T_B from the one-filament case is $0.27r^{1/2}$, and that the value of n_T^2 to reduce the enhancement to a half of its maximum value is also $0.27r^{1/2}$. Results approximately the same as these were mentioned in the previous section. Since the single-filament $T_B \propto (1/L)$, and $r^{1/2} \propto L$, Eq. (21) implies that T_B for large arrays is independent of L, provided n_L is large, but the number of filaments required to reach a given fraction of the maximum T_B is proportional to L.

From our numerical results in Figs. 1–3, we find that the enhancement factors at large n_T compared with the case $n_T = 1$ are equal to $r^{1/2}$ multiplied by about 0.30, 0.32, and 0.36 respectively, compared with the factor 0.27 predicted by Eq. (21). Defining a transverse bandwidth W_T by

$$W_T = 2\left(\hbar^2/2M_T\right)\left(\pi^2/a_T^2\right), \tag{22}$$

we find that the maximum value of $(k_B T_B/W_T)$ decreases from about 14 to 1.6 as we pass from parameters of Fig. 1 to those of Fig. 3. Thus we see that Eq. (21) is a better approximation for large n_T for larger values of this ratio, as we expected from our derivation [see Eq. (18)]. On the other hand the departure of the predictions of Eq. (21) below numerical values for small n_T is slightly larger for the parameters of Fig. 1, reaching 29.5% for $n_T = 4$ or 5 for these parameters, but only reaching 17% for $n_T \leq 5$ for the parameters of Fig. 3. This is presumably because of the relatively small value of $r^{1/2}$ (≈ 32) for the parameters of Fig. 1, which makes the approximations in deriving Eq. (20) have a bigger fractional effect on final results for any given small value of n_T.

According to Eq. (21), $k_B T_B$ saturates to a constant value for large n_T for given values of the other parameters. However, the numerical results of Figs. 1–3 show a slight fall for large n_T after a maximum is passed. We think this fall arises because, for L not sufficiently large compared with D, the quantity s of Eq. (13) will not be large, and so q of Eq. (15) will not be large for some small values of p_T. Then, for some p_T, the second term in the brackets of Eq. (16) will not be negligible. Hence, the sum will be lower than that found in the approximations appropriate for large length-to-width ratios, and so T_B will be lowered.

Now $cLE_L \propto (c/M_L L)$ and $r^{1/2} = (M_L/M_T)^{1/2}(L/a_T)$. Thus, for large n_T, Eq. (21) implies $T_B \propto (c/a_T)[1/(M_T M_L)^{1/2}]$. This differs from the result that $T_B \propto n^{2/3}(1/M_T^2 M_L)^{1/3}$, which occurs for anisotropic masses (for anisotropy which is not too extreme) [22] when bandwidths in all directions are large compared with $k_B T_B$; in this formula n is the three-dimensional carrier concentration, which is equivalent to (c/a_T^2) for our filament arrays. Presumably this difference arises because of our assumption that $W_T \ll k_B T_B$. In our numerical work we find a transition to this second type of dependence on masses when we decrease carrier concentrations or vary other parameters sufficiently to make the maximum transverse energy greater than the calculated T_B. For the value of values of c and a_T chosen for Figs. 1–3, this would only occur for values of $(M_T/M_L) < 1$, but for smaller values of c the transition occurs while $M_T > M_L$. This is illustrated in Fig. 4 where we show the ratio of $k_B T_B$ to the maximum transverse energy against M_L on a log–log plot for $cL = 200$ (i.e., ten times smaller than the value used for Figs. 1–3), values of (L/a_T) and n_L as before, and a value of n_T at which T_B reaches its maximum as a function of n_T. We do not use very large values of n_T in order to avoid the complications when s becomes small mentioned in the previous paragraph. For values of parameters used, n_T at which T_B is a maximum increases from 6 to about 220 as (M_L/M_T) increases from 10^{-4} to 1. In Fig. 4, we see most of a transition from a slope of $-1/2$ to a slope of $-1/3$ as (M_L/M_T) increases.

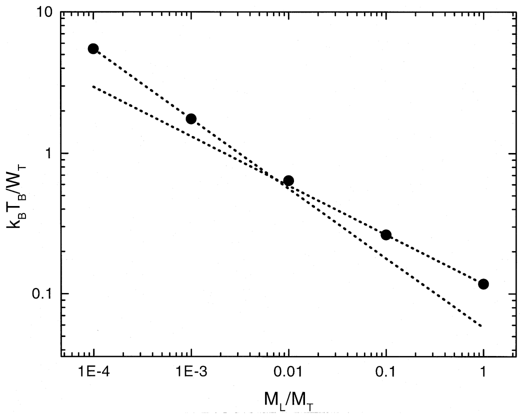

Fig. 4. Plot of maximum values with respect to n_T of $(k_B T_B / W_T)$, where W_T is the transverse bandwidth of Eq. (22), against (M_L / M_T) for $cL = 200$ and other parameters except masses as for Fig. 1. The figure shows most of a transition from a slope of $-1/2$ to a slope of $-1/3$ as the ratio $(k_B T_B / W_T)$ changes from about 5.5 to 0.12. The dotted lines illustrate the change of the average slope between the first two points and between the last two points from -0.49 to -0.35.

4. Conjectures about effects of disorder

Disorder can cause localisation of some states near the bottom of a band either for fermions or bosons [23,24]. The transition between localised and delocalised states occurs at a mobility edge E_c. When Coulomb interactions between bosons are taken into account, the bosons below the mobility edge behave more like fermions [24].

Let us consider the case for a filament array with $E_c < 3E_T$, the energy of the bottoms of the first excited bands with respect to transverse motion, and let us assume that the effects of disorder on states above E_c are unimportant. Then the only alterations of our previous calculations due to disorder will be (i) to replace the lower limits in the sum in Eq. (10) and in the sum for $i = j = 1$ in Eq. (3) by $k = k_c$, where k_c is the smallest value of k for which $E_L(k^2 - 1) > E_c$, and (ii) a generally small effect due to the fact that cLn_T^2 on the right-hand-side of Eq. (3) will be replaced by $[cLn_T^2 - (k_c - 1)]$, assuming only one boson can go in each localised state. With the change in the lower limit in Eq. (10) and the assumption that k_m is large, the right-hand side of Eq. (10) becomes approximately equal to $\{\frac{1}{2}[1/(k_c - 1) + 1/k_c](k_B T_B/E_L)\}$. Thus, as k_c increases above 2, the contribution of the states with minimum p_T to the overall sum of Eq. (3) becomes rapidly smaller, and so, in our approximate theory of Section 3, does the first term in the brackets in Eq. (19).

Since we are measuring our energies from a state of energy $(E_L + 2E_T)$ above the bottom of the bulk band, it is probable that, for a given amount of disorder, $(E_c + E_L + 2E_T)$ rather than E_c is independent of L. Thus, for a given channel width, D, there will be threshold length L below which no states will be localised. For L greater than this threshold, $E_c = K - E_L - 2E_T$, where K is a constant. Hence, if $K < 5E_T$, corresponding to our assumption that the mobility edge lies below the bottoms of the first excited subbands with respect to transverse motion, then k_c is the first integer greater than $z_c = [(K - E_L - 2E_T)/E_L]^{1/2}$. If $E_L \ll E_T$, this implies that k_c is approximately proportional to $L[K - C/n_T^2]$, where C is independent of L. Thus the term proportional to $(1/n_T^2)$ in the brackets in Eq. (19) or in the denominator of Eq. (21) is approximately proportional to $(1/L)$ for a given n_T. Since the second term in the denominator of Eq. (21) is also proportional to $(1/L)$, this means that the value of n_T to produce a given fractional reduction in T_B below its large n_T value does not change much with L after some states become localised for this n_T.

5. Conclusions

Numerical results for the Bose–Einstein condensation temperature T_B of a non-interacting Bose gas in a square array of filaments on a square lattice have been found for bosons characterised by masses M_L and M_T parallel and perpendicular to the filament directions, with cut-off wave vectors related to the lattice constant along a filament and to the filament separation, respectively. For large numbers of filaments, it has been shown that there is a gradual crossover from a proportionality of T_B to $(1/M_L M_T)^{1/2}$ to a proportionality to $(1/M_L M_T^2)^{1/3}$ as parameters are varied to make $k_B T_B$ change from being larger than to smaller than the maximum transverse boson energy, W_T. Approximate analytical expressions for T_B have been found for the case when W_T is small compared with $k_B T_B$. In the absence of disorder, the number of filaments required to give a condensation temperature equal to a given fraction of the limiting value for a large number of filaments is approximately proportional to $L(M_L/M_T)^{1/2}$ in this regime. It has been argued that disorder will act to flatten off any length dependence of this number above some length dependent on the amount of disorder.

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