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# The phase diagram of a two-dimensional array of mesoscopic granules

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**Abstract.** A lattice boson model is used to study ordering phenomena in regular 2D arrays of superconductive mesoscopic granules, Josephson junctions and pores filled with superfluid helium. The phase diagram of the system, for when quantum fluctuations of both the phase and the local superfluid density are essential, is analysed both analytically and by the quantum Monte Carlo technique. For the system of strongly interacting bosons it is found that as the boson density  $n_0$  is increased the boundary of the ordered superconducting state shifts to *lower temperatures* and at  $n_0 > 8$  approaches its limiting position corresponding to negligible relative fluctuations of the moduli of the order parameter (as in an array of ‘macroscopic’ granules). In the region of weak quantum fluctuations of phases, mesoscopic phenomena manifest themselves up to  $n_0 \sim 10$ . The mean-field theory and functional integral ( $1/n_0$ )-expansion results are shown to agree with those of quantum Monte Carlo calculations of the boson Hubbard model and its quasiclassical limit, the quantum  $XY$ -model.

## 1. Introduction

The study of mesoscopic systems has already led to many new interesting fundamental concepts [1, 2]. Progress has been especially rapid due to the development of nanotechnology methods which has opened up new avenues for sophisticated experiments. In this connection the study of arrays of ultrasmall granules, microclusters and Josephson junctions is of particular concern (see e.g. [3, 4]).

Granular superconductors, Josephson arrays and superfluid helium in porous media [5] are, as a rule, described in terms of different modifications of the quantum  $XY$ -model (see below), but this description is correct only if the relative fluctuations of the local superfluid density are not essential [6]. Such fluctuations take place in sufficiently large granules at temperatures far below that of the onset of superconductivity in each individual granule. To study the role of quantum fluctuations of moduli other more appropriate models should be used.

A convenient starting point for the description of the  $N \times N$  system of interacting bosons (Cooper pairs in granules, He atoms in pores etc) is the Bose–Hubbard Hamiltonian:

$$\hat{H}_H = \frac{t}{2} \sum_{\langle i, j \rangle} \left\{ 2a_i^\dagger a_i - a_i^\dagger a_j - a_j^\dagger a_i \right\} + \frac{U}{2} \sum_i \left\{ a_i^\dagger a_i - n_0 \right\}^2 \quad (1)$$

where  $a_i^\dagger$  ( $a_i$ ) is a boson creation (annihilation) operator at a site  $i = \overline{1, N^2}$ ;  $t$  is the strength of the hopping between nearest-neighbour sites  $\langle i, j \rangle$  and  $U > 0$  is an on-site repulsive interaction.

The system (1) has a rich phase diagram [7, 8], containing a Mott insulating phase (at zero temperature) and the superfluid and normal (metal) phases. At a commensurate density  $n_0 = \langle a_i^\dagger a_i \rangle$  (the number of bosons is an integer multiple of the number of sites) and  $T = 0$ , the boson Hubbard model lies in the same universality class (see [7–9]) as the quantum XY-model with the Hamiltonian

$$\hat{H}_{XY} = J \sum_{\langle i,j \rangle} \{1 - \cos(\varphi_i - \varphi_j)\} - \frac{U}{2} \sum_i \{\partial/\partial\varphi_i\}^2 \quad (2)$$

where the  $\varphi_i \in [0, 2\pi)$  are phases of the order parameter. Obviously, at  $T \neq 0$  the requirement for the density to be commensurate,  $n_0 = k$ , is too stringent. In the latter case, the behaviour of the system (1) will depend *continuously* on  $n_0$ , and the *critical* properties will be *the same* in some band  $n_0 = k \pm \delta n_0$ ; the width  $2\delta n_0$  should decrease as the temperature is lowered.

The properties of the system (2), which exhibits at finite temperatures superfluid and metallic phases, are described by two dimensionless parameters: the temperature in units of the Josephson coupling constant  $T = k_b T/J$  and the quantum parameter  $q = \sqrt{U/J}$  which is responsible for the strength of the zero-point fluctuations of the phase. The corresponding parameters of the Hubbard model are  $T = k_b T/(tn_0)$  and  $q = \sqrt{U/(tn_0)}$ .

The general aim of this communication is that of comparing the phase diagrams of models (1) and (2) in order to estimate the importance of the mesoscopic phenomena in regular 2D systems. Of prime interest to us is the case of *finite temperatures*, together with the intriguing quantum phase transitions which take place at  $T = 0$  (see e.g. [10] and references therein). Sections 2 and 3 present the mean-field and functional integral ( $1/n_0$ )-expansion approaches. From *ab initio* quantum Monte Carlo calculations of different characteristic quantities (section 4) we determine the phase diagram  $T_H^c(q; n_0)$  of the boson Hubbard model at different densities  $n_0$  and compare it (section 5) with the phase diagram of the 2D quantum XY-model.

## 2. Mean-field approximation

A qualitative estimation of the phase diagram of the boson model (1) can be obtained in a simple mean-field approximation (see e.g. [11–13] and references therein). The boundary  $T^c(q; n_0)$  of the ordered state can be found in the MFA from the equation

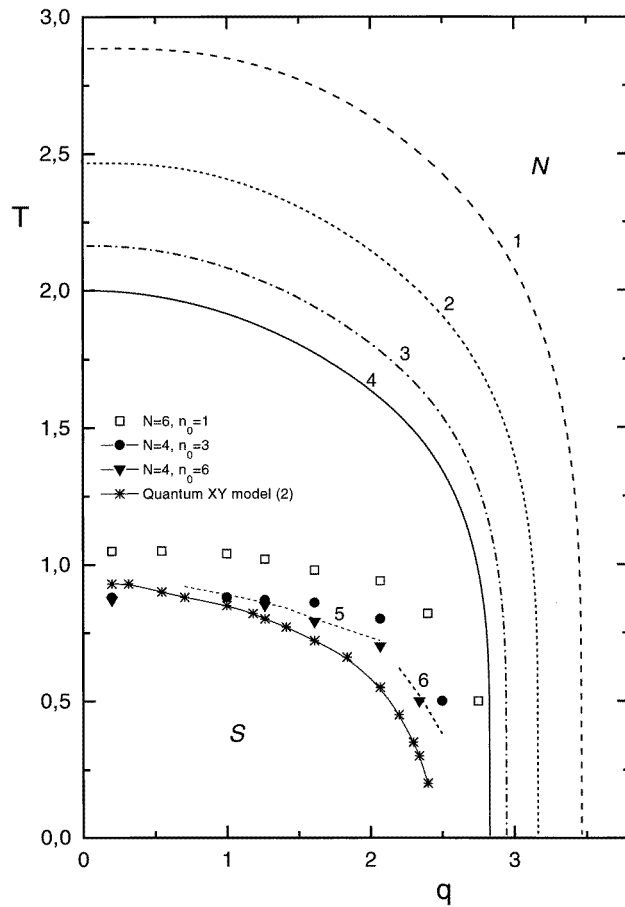
$$\frac{q^2}{z} = \left( \sum_{n=-n_0}^{\infty} \{n + n_0 + 1\} \left\{ e^{-q^2[n-\eta]^2/(2T)} - e^{-q^2[n+1-\eta]^2/(2T)} \right\} / \{2n + 1 - 2\eta\} \right) \times \left( n_0 \sum_{n=-n_0}^{\infty} e^{-q^2(n-\eta)^2/(2T)} \right)^{-1} \quad (3)$$

where  $\eta = \mu/U - z/(2q^2 n_0)$  and  $z$  is the number of nearest neighbours ( $z = 4$  for a 2D square lattice). Equation (3) for the boundary of the ordered state differs in some details from that of reference [12]. The two equations become equivalent in the limit of large densities  $n_0$ , with equation (3) being more accurate for  $n_0 \sim 1$ .

The condition for the chemical potential  $\mu$  is that the mean number of particles must be equal to  $n_0$ :

$$\sum_{n=-n_0}^{\infty} n \exp(-q^2\{n - \eta\}^2/(2T)) = 0. \quad (4)$$

It should be pointed out that in the limit  $n_0 \rightarrow \infty$ , equation (4) gives  $\mu = 0$  and the boundary of the ordered state transforms to that of the quantum  $XY$ -model [11].



**Figure 1.** The phase diagram of the 2D Hubbard model (1) and the quantum  $XY$ -model (2). S: superconducting; N: normal state. The mean-field results: **1**:  $n_0 = 1$ ; **2**:  $n_0 = 2$ ; **3**:  $n_0 = 6$ ; **4**: the quantum  $XY$ -model ( $n_0 = \infty$ ). The  $(1/n_0)$ -expansion (8) results: **5**:  $n_0 = 6$ ; **6**:  $n_0 = 14$ . Symbols indicate points where phase transitions have been found by the MC method.

The lines  $T_H^c(q; n_0)$  of the boson Hubbard model obtained from equations (3) and (4) are shown in figure 1 for different densities  $n_0$ . Calculation shows that the lines  $T_H^c(q; n_0)$  reach their limiting position, the phase boundary  $T_{XY}^c(q)$  of the quantum  $XY$ -model, at  $n_0 > 25$ .

### 3. The $(1/n_0)$ -expansion

To improve the qualitative mean-field estimation of the difference of the phase diagrams of models (1) and (2), let us represent the partition function of the Hamiltonian (1) in a path

integral representation as a trace over a complex  $c$ -number Bose field  $\Phi$  [9]:

$$Z_H = \text{tr} \{e^{-S}\} = \int D(\Phi, \Phi^*) e^{-S(\Phi, \Phi^*)}$$

$$S(\Phi, \Phi^*) = \int_0^\beta \left\{ i \sum_i \dot{\Phi}_i \Phi_i^* + \frac{t}{2} \sum_{(i,j)} |\Phi_i - \Phi_j|^2 + \frac{U}{2} \sum_i [|\Phi_i|^2 - n_0]^2 \right\} d\tau \quad (5)$$

$$\Phi_i(0) = \Phi_i(\beta)$$

$$\Phi_i^*(0) = \Phi_i^*(\beta).$$

Substituting  $\Phi_i = \sqrt{n_0 + \delta n_i} e^{i\varphi_i}$  (for integer  $n_0$ ) in equation (5) gives

$$Z_H = \int D(\delta n, \varphi) e^{-S(\delta n, \varphi)}$$

$$S(\delta n, \varphi) = \int_0^\beta \left\{ \frac{U}{2} \sum_i [\delta n_i]^2 + i \sum_i \delta n_i \dot{\varphi}_i + t n_0 \sum_{(i,j)} \left[ 1 + \frac{\delta n_i + \delta n_j}{2n_0} - \sqrt{(1 + \delta n_i/n_0)(1 + \delta n_j/n_0)} \cos(\varphi_i - \varphi_j) \right] \right\} d\tau \quad (6)$$

$$\delta n_i \equiv n_i - n_0 = \delta n_i(\tau)$$

$$\varphi_i = \varphi_i(\tau).$$

From equation (6) one can see that increasing the mean number of particles at each granule, provided that  $J = t n_0$  and  $U$  are constant, enables one to leave the action in terms of the phase degrees of freedom unchanged [6, 9]. This leads to the action of the quantum  $XY$ -model.

As we are interested in the difference between the phase boundaries of models (1) and (2) at sufficiently high but finite  $n_0$ , let us expand the superfluid density in powers of  $1/n_0$  up to second order. Defining the superfluid density on the basis of the response of a system to the shift of phases at the boundary [14], from equation (6) we have

$$\nu_s = \gamma + \frac{1}{2n_0^2} \Gamma^{(2)} + \dots \quad (7)$$

where  $\gamma$  is the helicity modulus of the quantum  $XY$ -model [15, 16]. The first-order corrections are equal to zero due to the invariance of the action of the  $XY$ -model under 'time' inversion.

The rather complex expression for  $\Gamma^{(2)}$  can be represented as some equilibrium value of the quantum  $XY$ -model [13], which can be easily estimated via the quantum Monte Carlo technique or one of the self-consistent approximations [17].

Given a value of the coefficient  $\Gamma^{(2)}$  in the expansion (7) as a function of the control parameters,  $\Gamma^{(2)} = \Gamma^{(2)}(q, T)$ , one can construct an upper estimate for the phase boundary  $T_H^c(q; n_0)$  of the boson Hubbard model (1):

$$T_H^c(q; n_0) \leq T_{XY}^c(q) \left\{ 1 + \frac{\nu_s(q, T_{XY}^c) - \gamma(q, T_{XY}^c)}{\gamma(q, T_{XY}^c)} \right\} = T_{XY}^c(q) \left\{ 1 + \frac{\pi \Gamma^{(2)}(q, T_{XY}^c)}{4n_0^2 T_{XY}^c(q)} \right\} \quad (8)$$

where  $T_{XY}^c(q)$  is the line of topological phase transitions of the quantum  $XY$ -model (2). The estimate (8) can be easily obtained from the assumption that the lines of phase transitions of both models are defined by the universal relation [15]

$$\gamma(q, T_{XY}^c) = 2T_{XY}^c/\pi \quad \nu_s(q, T_H^c) = 2T_H^c/\pi.$$

The results of the above-mentioned estimations are given in figure 1. It turns out that in the region  $0.7 < q < 1.5$  the line of phase transitions of the Hubbard model approaches (to within 5%) its limit at  $n_0 = 8$ , whereas some greater densities  $n_0 > 16$  are required in the strongly quantum region  $q > 1.7$  because of the rapid increase of the coefficient  $\Gamma^{(2)}(q)$ . Direct Monte Carlo calculation of the phase diagram  $T_H^c(q)$  (see below), which is in agreement with the predictions of the  $(1/n_0)$ -expansion for  $0.7 < q < 1.5$ , shows that in the case of a *strongly* interacting system (at  $q > 1.7$ ) theoretical estimations markedly overestimate the maximum boson density  $n_0$  at which mesoscopic effects are still essential.

To conclude this section, one additional feature should be recognized. It is easy to see that all of the estimations presented in this section and starting from the partition function (5) have been carried out in the *grand canonical* ensemble with zero chemical potential. This has enabled us to make all of the calculations analytically, disregarding the restrictions on the total number of particles in the system when integrating over the fluctuations of the moduli of the order parameter. In order to justify comparing MC results with theoretical estimations, we need to show that, when calculated within the  $(1/n_0)$ -expansion, the discrepancy  $\delta n$  between the mean number of bosons per granule and  $n_0$  is small.

From the expression given in (6) for  $\delta n$ , one can write

$$\delta n = \frac{1}{n_0} \Delta^{(1)} + \dots \tag{9}$$

As calculation shows, the value of  $\Delta^{(1)}$  is less than 0.1 in the region  $q > 0.7$ ,  $T < 1$ . This observation justifies our use of the grand canonical ensemble with zero chemical potential in estimating the coefficient  $\Gamma^{(2)}$  of the series (7).

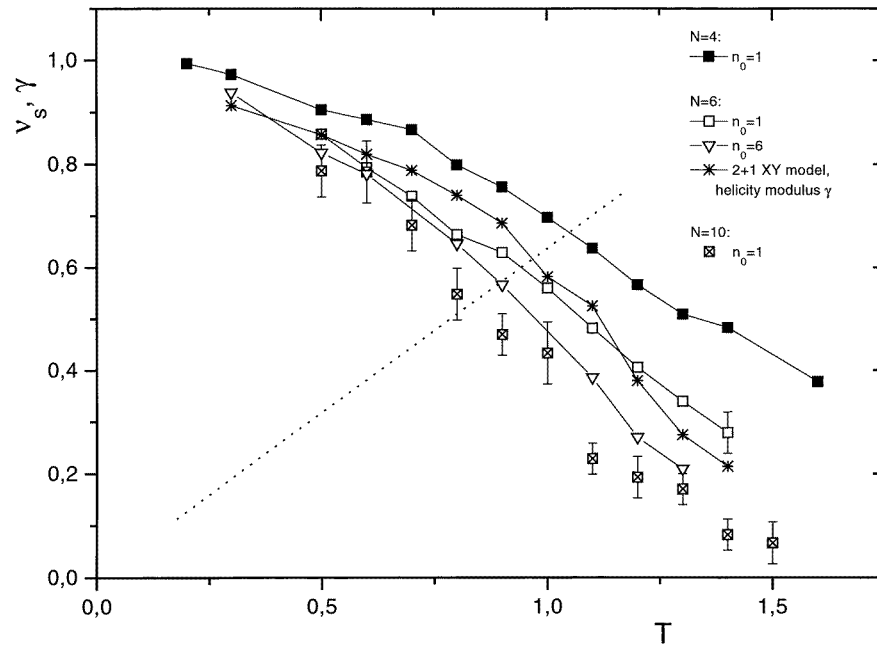
#### 4. Quantum Monte Carlo simulations

In studies of properties of the boson Hubbard model (1) at different values of the control parameters  $\{q, T\}$  we have applied the ‘chequerboard’ break-up [18]. In this method the classical degrees of freedom to be sampled are the imaginary-time-dependent boson occupation number field  $\{n_i^p\}$ ,  $i = 1, \dots, N^2$ ,  $p = 0, \dots, 4P$ . The algorithm of the Monte Carlo (MC) calculations of the quantum *XY*-model was described in [16, 19]. We have performed extensive tests to verify that our results converge in the limit  $P \rightarrow \infty$ . The results presented below have been obtained by the averaging over 3–5 initial configurations formed by multiplication by  $4P$  (by  $P$  for the *XY*-model) of the random configuration of bosons (phases for the *XY*-model) in the  $N \times N$  lattice.

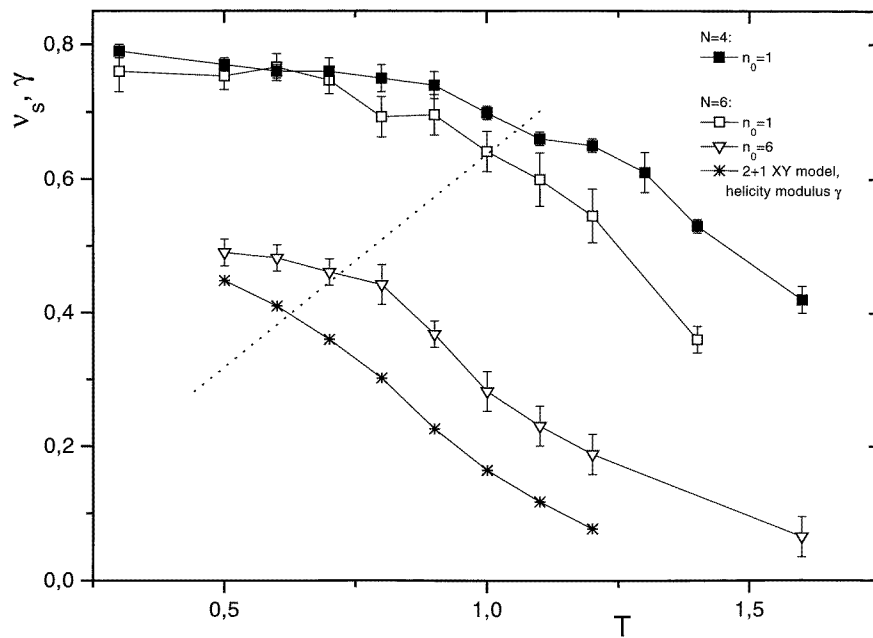
The main focus of attention has been the calculation of the superfluid density  $\nu_s$ . This quantity has been determined from the winding number [8, 18]:

$$\begin{aligned} \nu_s &= 0.5T \langle W_x^2 + W_y^2 \rangle_H \\ W_x &= \sum_{p=0}^{4P} \sum_{i_y=1}^N (-1)^{i_x+p} n_i^p \\ W_y &= \sum_{p=0}^{4P} \sum_{i_x=1}^N (-1)^{i_y+p} n_i^p \end{aligned} \tag{10}$$

where  $n_i^p$  means the number of bosons at a site  $i$  (with coordinates  $\{i_x, i_y\}$ ) at the level  $p$



(a)



(b)

**Figure 2.** (a) The superfluid density  $v_s$  (the helicity modulus  $\gamma$ ) versus temperature  $T$  at  $q = 0.2$ . The dependence  $2T/\pi$  (see the text) is given by a dashed line. The data are connected to guide the eyes. If not present, error bars are smaller than the size of the data point. (b) The superfluid density  $v_s$  (the helicity modulus  $\gamma$ ) versus temperature  $T$  at  $q = 2.0$ .

of a 3D classical system. We have also used the current autocorrelation function [20]:

$$\begin{aligned}
 v_s &= -\frac{1}{n_0 N^2} \langle \hat{T}_x \rangle_H - \frac{1}{n_0^2 N^2 T P} \sum_{\tau=0}^{P-1} \left\langle \hat{J}_x^{(p)}(\tau) \hat{J}_x^{(p)}(0) \right\rangle_H \\
 \hat{T}_x &= -\frac{1}{2} \sum_i \left\{ a_{i+x}^\dagger a_i + a_i^\dagger a_{i+x} \right\} \\
 \hat{J}_x^{(p)} &= -\frac{i}{2} \sum_i \left\{ a_{i+x}^\dagger a_i - a_i^\dagger a_{i+x} \right\} \\
 \hat{J}_x^{(p)}(\tau) &= e^{\tau \beta \hat{H}/P} \hat{J}_x^{(p)} e^{-\tau \beta \hat{H}/P}.
 \end{aligned} \tag{11}$$

The substitution  $a_i \rightarrow \sqrt{n_0} e^{i\varphi_i}$  transforms equation (11) to the well-known expression for the helicity modulus  $\gamma$  of the quantum  $XY$ -model [16].

As has been pointed out by Scalapino and co-workers [21], the temperature derivative of the superfluid density gives additional information about the type of phase transition at some temperature  $T^c(q)$ : in the framework of the Kosterlitz–Thouless picture, the value of  $\partial(\beta v_s)/\partial\beta$  scales as a Dirac delta function  $\delta(T - T^c)$ . On finite lattices,  $\partial(\beta v_s)/\partial\beta$  shows a response which increases with lattice size  $N$ , the position of the maximum of the derivative being independent of  $N$ .

To find the derivative of the superfluid density  $\partial(\beta v_s)/\partial\beta$  we have estimated the difference in internal energies of systems which differ by a phase twist  $\delta\varphi$  in the boundary condition along one lattice direction:

$$\frac{\beta \{E(\delta\varphi) - E(0)\}}{n_0 \beta t} \sim v_s + \beta \frac{\partial v_s}{\partial \beta}. \tag{12}$$

One can show that for the Cooper pairs of charge  $2e$  this phase twist can be realized in the ‘flux quantization’ scheme and is equivalent to threading a flux through the centre of a torus on which the system lies [21].

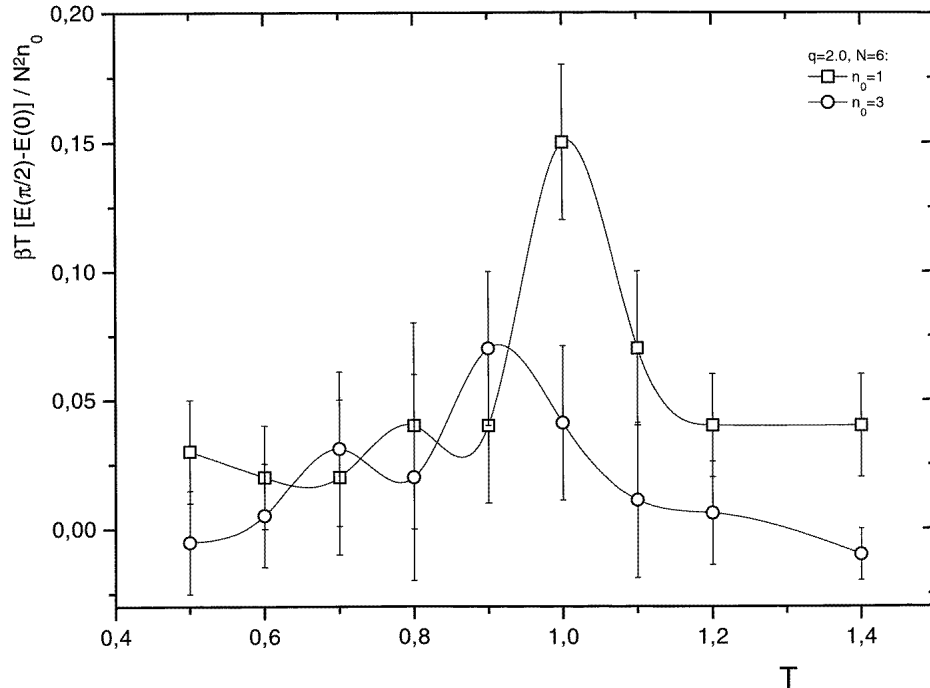
We have also calculated the fluctuation of bosons at lattice sites:

$$\delta n_H^2 = \frac{1}{4PN^2} \left\langle \sum_{p=0}^{4P-1} \sum_i \{n_i^p - n_0\}^2 \right\rangle_H. \tag{13}$$

### 5. Results and discussion

Shown in figure 2 are the dependencies of the superfluid fraction  $v_s(T)$  of the Hubbard model at  $q = 0.2$  (in the classical region of the  $XY$ -model (2); see figure 2(a)) and  $q = 2.0$  (see figure 2(b)). For reference, the helicity modulus  $\gamma$  of the quantum  $XY$ -model as a function of temperature  $T$  is also plotted. Analysis of data obtained at different sizes  $N$  and densities  $n_0$  of the system reveals that for a system of strongly interacting bosons (at  $q = 2.0$ ) the MC results are in qualitative agreement with the theoretical estimations of sections 2 and 3. In fact, from figures 1 and 2 one can see that as the density of bosons  $n_0$  is increased, the boundary of the ordered superconducting state of the system (1) approaches that of the quantum  $XY$ -model with the critical temperatures  $T_H^c$  of the Hubbard model being greater than that,  $T_{XY}^c$ , of the quantum  $XY$ -model. The line of transitions  $T^c(q)$  can be estimated from the universal relation  $v_s(T^c) = 2T^c/\pi$ . Thus defined, the temperature of the metal–superconductor transition agrees fairly well with the position of the peak of the temperature derivative of the superfluid density (12). Our calculation shows that the





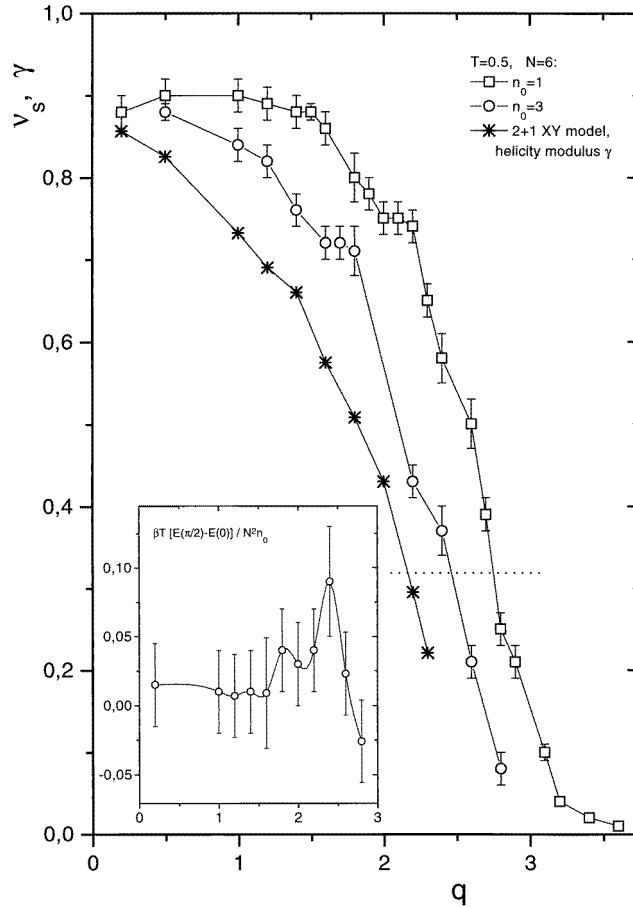
**Figure 3.**  $T\beta\{E(\pi/2) - E(0)\}/\{n_0N^2\}$  as a function of temperature  $T$ . The solid lines are spline fits to the data.

position of the maximum of the derivative does not depend (within statistical errors) on the system size and, as one can see from figure 3, shifts to lower values of  $T$  as  $n_0$  is increased.

From figure 2(a) one can see that the transition temperature of the weakly interacting bosons (at  $q = 0.2$ ) appears to be *less* than that of the quantum  $XY$ -model. This tendency persists with increasing system size. The theoretical approach used in section 3 cannot help to elucidate the reasons for this phenomenon, because at  $q < 0.4$  the relative fluctuations of the moduli of the order parameter are only weakly damped by the interaction, the corrections  $\Gamma^{(2)}$  and  $\Delta^{(1)}$  are large and the theoretical estimations are inaccurate.

Let us consider the behaviour of  $\nu_s(q)$  and  $\gamma(q)$  as functions of the quantum parameter  $q$  at  $T = 0.5$  (see figure 4). Defining the point  $q^c$  of the phase transition on the basis of the universal relation  $\nu_s(q) = 2T/\pi$ , we see that the boundary of the ordered superconducting state of the model (1) lies to the right of the boundary of the model (2). This conclusion is verified by the results of the calculations of the derivative  $\partial(\beta\nu_s)/\partial\beta$  presented in the inset in figure 4. The position  $q|_{n_0=3} \approx 2.3$  of a peak of the derivative is in fairly good agreement with the critical point  $q^c|_{n_0=3} \approx 2.4$  determined from the universal relation.

The dependence of the relative fluctuations of the particle number at sites of the system versus the quantum parameter  $q$  is shown in figure 5. In particular, figure 5 can serve as an illustration of the role of interaction in the transition to the quasiclassical limit from the boson Hubbard model to the quantum  $XY$ -model. In fact, at finite densities  $n_0$ , the spectrum of the operator  $\hat{n}_i - n_0$  can be considered as unbounded only if the relative fluctuations of the particle number are small,  $\delta n_H^2/n_0^2 \ll 1$ . Then, as is usually done by examination of Josephson or granular systems in terms of the model (2), the particle number operator  $\hat{n}_i - n_0$  can be chosen as one conjugate to the 'phase' operator  $\hat{\varphi}_i$ :  $\hat{n}_i - n_0 = i\partial/\partial\varphi_i$ .

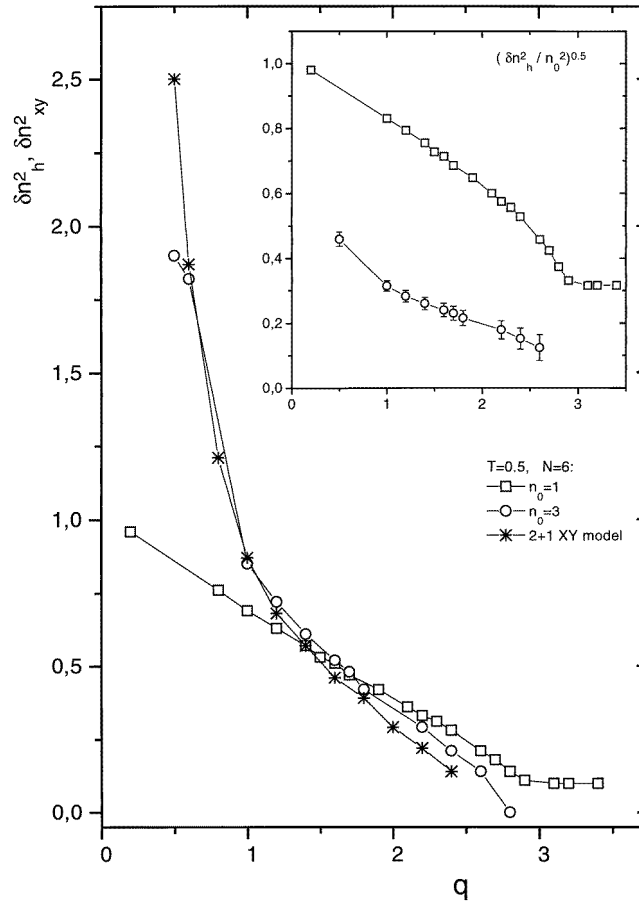


**Figure 4.** The superfluid density  $v_s$  (the helicity modulus  $\gamma$ ) versus the quantum parameter  $q$  at  $T = 0.5$ . The line  $1/\pi$  is shown with the help of a dashed line. Inset: the temperature derivative of the superfluid fraction (12).

Increasing of the strength of the interaction (quantum parameter  $q$ ) leads to the suppression of the relative fluctuations of the order parameter modulus as can be seen from figure 5. It should be noted that at high  $q$  the fluctuations of the particle number are *greater* than those of the quantum  $XY$ -model, but they become more similar with increase in density. The results presented in the inset of the figure are relative fluctuations  $\delta n_H^2/n_0^2$  as functions of the quantum parameter  $q$  at  $T = 0.5$  at different densities  $n_0$ . The increase in  $n_0$  is seen to be of great importance in suppressing the relative fluctuations.

Great attention has been paid thus far to the possibility of *re-entrance* phenomena, when the global superconducting state in some region of  $q$  is absent not only at high, but also at sufficiently low temperatures. In the framework of the  $XY$ -model the possibility of this phenomenon taking place has been connected with the domain of phases [11], dissipation or mutual capacitance effects [22, 23]. From the results presented, one can see that taking into account the fluctuation of the moduli of the order parameter does not lead to re-entrance phenomena at least in the region explored.

To conclude, we have used the boson Hubbard model to analyse the effect of quantum



**Figure 5.** The fluctuation  $\delta n_H^2$  of the number of bosons at sites of the system as a function of the quantum parameter  $q$  at  $T = 0.5$ . Inset: the relative fluctuations  $\delta n_H^2/n_0^2$  at different densities  $n_0$ .

fluctuations of phases and moduli of the order parameter on the onset of superconductivity in a 2D mesoscopic Josephson system. Both mean-field approximation and  $(1/n_0)$ -expansion lead to the conclusion that the line  $T^c(q)$  of superconductor–metal phase transitions lies *above* that of the quantum  $XY$ -model, the latter being the quasiclassical limit (as  $n_0 \rightarrow \infty$ ;  $U \neq 0$ ) of the Hubbard one. Our MC simulations show that in the region  $q < 1$  of small quantum fluctuations of phases it needs an average of ten bosons per site to suppress relative fluctuations of the local superfluid density. As the strength of the interaction is increased, the quasiclassical limit is approached at lower densities ( $n_0 \sim 8$  at  $q \sim 2$ ). No re-entrance or discontinuity phenomena have been found.

### Acknowledgments

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