Interacting bose gas in an optical lattice

Klaus G. Ziegler

Interacting Bose Gas in an Optical Lattice[*]

K. Ziegler

Institut für Physik, Universität Augsburg, Germany

E-mail: klaus.ziegler@physik.uni-augsburg.de

A grand canonical system of hard-core bosons in an optical lattice is considered. The bosons can occupy randomly N equivalent states at each lattice site. The limit $N \to \infty$ is solved exactly in terms of a saddle-point integration, representing a weakly-interacting Bose gas. In the limit $N \to \infty$ there is only a condensate if the fugacity of the Bose gas is larger than 1. Corrections in $1/N$ increase the total density of bosons but suppress the condensate. This indicates a depletion of the condensate due to increasing interaction at finite values of N.

1. INTRODUCTION

Recently developed systems of trapped ultra-cold gases open a wide new field for the study of many-particle physics.[1] This includes the investigation of Bose-Einstein condensation of interacting Bose particles[2,3], leading to macroscopic quantum states or "matter waves". Among the most interesting experiments there is the trapping of bosons in so-called optical lattices[4-6] that are created by intersecting Laser fields. Typical lattice constant of optical lattices are $a_l = 250...500$nm. They exhibit unsual properties due to the interference of macroscopic quantum states. The interaction between the atoms is characterized by the ratio of the scattering length a and the typical particle distance $n^{-1/3}$ as $an^{1/3}$, where n is density of particles. In most of the experiments we have $an^{1/3} < 10^{-2}$ such that these systems are dilute[1]. Interaction plays only a weak role in these systems such that the Gross-Pitaevskii approach is sufficient[7,8]. After the experimental discovery of Feshbach resonances in the trapped Bose gases it became possible to tune the inter-atomic interaction with an applied magnetic field over a wide range

---

[*]Dedicated to Peter Wölfle on the occasion of his 60th birthday.

of interactions[9–11]. The scattering length for [85]Rb atoms is $a \approx 5$nm but near Feshbach resonances it is up to 500nm[11]. In this case one can study an optical lattice in which the lattice constant (determined by the wave length of the applied Laser field) is equal to the scattering length. Then at most one boson can be found in the minima of the optical lattice.

From the theoretical point of view this field requires the study of models with strongly interacting particles. The so-called Bose-Hubbard model has been used[4,5] to decribe an on-site interaction with coupling strength U. A mean-field calculation[5] has shown that the condensate vanishes in the strong-coupling limit $U \to \infty$, indicating that a strong interaction among the bosons has a destructive effect on the condensate. On the other hand, from the experiments it is believed that the interaction can still be considered as hard-core, characterized only by the scattering length a but including many-particle collisions.

In the following we will tune the interaction by going from the weakly interacting (dilute) to the strongly interacting hard-core Bose gas. This will be achieved by the assumption that each lattice site can accommodate N bosons with the same energy[12]. Bosons can randomly change between these states and tunnel between neighboring lattice sites from/to any of these N bosonic states with the same rate. Interaction exists only between bosons at the same state. The regime $N \gg 1$ describes a dilute Bose gas whereas $N = 1$ corresponds to a hard-core Bose gas with only one state per lattice site. We will solve the limit $N \to \infty$ within a saddle-point integration and apply a $1/N$-expansion to control systematically the corrections to the dilute Bose gas towards a more strongly interacting bosons.

2. BOSONS IN AN OPTICAL LATTICE

In the first part of this section the Bose gas on a lattice will be discussed without interaction using a complex field ϕ. This field will be replaced in the second part by a hard-core field which has the same propagator as the field ϕ. Therefore, in contrast to the Bose-Hubbard model, the interaction is carried by the field and not directly by the Hamiltonian. A model of non-interacting bosons is considered on a d-dimensional hypercubic lattice with $\mathcal{N}$ sites. A boson can occupy statistically one of N degenerate states at each site, and tunneling between these N states at lattice site r to any of the states at site r' occurs with the rate $J_{r,r'}^{\alpha,\alpha'}$. This is represented by the Hamiltonian

$$\hat{H} = -\frac{1}{2} \sum_{\alpha,\alpha'=1}^{N} \sum_{r,r'} J_{r,r'}^{\alpha,\alpha'} \Phi_r^{+\alpha} \Phi_{r'}^{\alpha'} \tag{1}$$

with bosonic creation and annihilation operators $\Phi_r^{+\alpha}$, $\Phi_{r'}^{\alpha'}$. The statistics of a system of bosons can be described by introducing a grand-canonical ensemble with fugacity ζ at the inverse temperature β. In the case of non-interacting bosons it is defined by the partition function[3]

$$Z = \prod_j \frac{1}{1 - \zeta^\beta e^{-\beta \epsilon_j}}, \tag{2}$$

where ϵ_j are the eigenvalues of the Hamiltonian matrix

$$H_{r,r'}^{\alpha,\alpha'} = -\frac{1}{2} J_{r,r'}^{\alpha,\alpha'} .$$

Assuming that β has integer values, the factors in Eq. (2) can be expressed by the determinant of a $\beta \times \beta$–matrix as

$$1 - \zeta^\beta e^{-\beta \epsilon_j} = \det(\mathbf{1} - \zeta w_j),$$

where

$$w_j = \begin{pmatrix} 0 & u & 0 & \dots & 0 \\ 0 & 0 & u & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 0 & u \\ u & 0 & \dots & 0 & 0 \end{pmatrix} \quad \text{with} \quad u = e^{-\epsilon_j}. \tag{3}$$

Then the partition function can also be written as the determinant of a $\beta \mathcal{N} \times \beta \mathcal{N}$–matrix as

$$Z = \frac{1}{\det(\mathbf{1} - \zeta \hat{w})}. \tag{4}$$

$\hat{w}$ is obtained from expression (3) by using for u the $\mathcal{N} \times \mathcal{N}$–matrix $u = e^{-H}$. It is convenient for the following to introduce space-time coordinates $x = (t, r)$ with a "time" variable $t = 1, 2, ..., \beta$. Moreover, we assume that the matrix $H = -\log u$ is chosen such that

$$\hat{w}_{x,x'}^{\alpha,\alpha'} = \frac{1}{N} w_{x,x'}. \tag{5}$$

2.1. Random-Walk Expansion

Using a complex field ϕ_x the inverse determinant in Eq. (4) reads

$$Z = \int \exp\left[-\sum_x \sum_{\alpha=1}^N \bar{\phi}_x^\alpha \phi_x^\alpha + \frac{\zeta}{N} \sum_{x,x'} \sum_{\alpha,\alpha'=1}^N w_{x,x'} \bar{\phi}_x^\alpha \phi_{x'}^{\alpha'} \right] \prod_x d\bar{\phi}_x^\alpha d\phi_x^\alpha / \pi. \tag{6}$$

The field is subject to periodic boundary conditions in t

$$\phi_{\beta+1,r}^{\alpha} = \phi_{1,r}^{\alpha}. \tag{7}$$

The integrand of Z in the expression (6) can be formally expanded in powers of the matrix w as

$$\exp\left(\frac{\zeta}{N}\sum_{x,x'}\sum_{\alpha,\alpha'=1}^{N} w_{x,x'}\bar{\phi}_x^{\alpha}\phi_{x'}^{\alpha'}\right) = \prod_{t=1}^{\beta}\prod_{r,r'}\prod_{\alpha,\alpha'=1}^{N}\left(\sum_{l\geq 0}\frac{1}{l!}[\frac{\zeta}{N}u_{r,r'}\bar{\phi}_{t,r}^{\alpha}\phi_{t+1,r'}^{\alpha'}]^l\right). \tag{8}$$

The integration over the Bose field ϕ_x can be performed for each expansion term, leading to a random-walk expansion of Z with elements $\zeta u_{r,r'}$.[12,14] From Z we can evaluate the density of bosons as

$$n = \frac{\zeta}{\mathcal{N}N\beta}\frac{\partial}{\partial\zeta}\log Z. \tag{9}$$

In the case of the non-interacting Bose gas Eq. (2) we get immediately

$$n = -1 + \frac{1}{\mathcal{N}N\beta}\text{Tr}[(\mathbf{1} - \zeta w/N)^{-1}] = \frac{1}{\mathcal{N}N\beta}\sum_{l\geq 1}\left(\frac{\zeta}{N}\right)^l\text{Tr}(w^l).$$

w^l contains $l-1$ summations with respect to $\alpha = 1, ..., N$, contributing a factor N^{l-1}. Another factor N comes from the trace. Altogether, this gives $n \propto N^{-1}$, a consequence of the scaling in Eq. (5). It should be noticed that ζ is restricted here to $\zeta \leq 1$ if the eigenvalues of w/N are ≤ 1. This is a well-known artefact of non-interacting bosons[3]. As we will see subsequently, $\zeta \geq 0$ is not restricted in the interacting Bose gas and has a non-zero density for $\zeta > 1$ even in the limit $N \to \infty$.

2.2. The Hard-Core Bose Gas

A hard-core condition can now be implemented in this model by assuming that a crossing of different random walks is prohibited. For this purpose it is useful to return to Eq. (8). It has been shown[12] that the statistics of the directed lines with hard-core interaction can be described conveniently by replacing the complex field ϕ_x^{α} by a field constructed from an algebra of nilpotent numbers (i.e., $(\eta_x^{\alpha,\sigma})^l = 0$ if $l > 1$):

$$\phi_x^{\alpha} \to \eta_x^{\alpha,\sigma} \quad (\sigma = \pm 1).$$

Each space-time point x is characterized by quantum numbers (α, σ), where $\sigma = \pm 1$ corresponds to the real and the imaginary part of ϕ_x^{α}. This choice

implies $2N$ degrees of freedom at each point x. Therefore, we need also $2N$ variables $\eta_x^{\alpha,\sigma}$ at x. Since $\{\eta_x^{\alpha,\sigma}\}$ are nilpotent, we have an exclusion principle describing the hard-core interaction. Products of $\eta_x^{\alpha,\sigma}$ must be commutative in order to represent the Bose statistics. Now one can identify an empty site with

$$\eta_x^{\alpha,1}\eta_x^{\alpha,2}.$$

and a tunneling process, going from x to x' and connecting the states α and α', with

$$\frac{\zeta}{N}w_{x,x'}\eta_x^{\alpha,1}\eta_{x'}^{\alpha',2},$$

where $w_{x,x'}$ $(= w_{x-x'})$ describes again the hopping probability as obtained from the random-walk expansion.

The integration over the free Bose field ϕ is replaced by a linear mapping of the algebra, generated by $\{\eta_x^{\alpha,\sigma}\}$, to the complex numbers with

$$\int_{HC} \prod_{x \in \Lambda' \subseteq \Lambda} \prod_{\alpha \in i_x} \prod_{\sigma \in j_{x,\alpha}} \eta_x^{\alpha,\sigma} = \begin{cases} 1 & \text{if } \Lambda' = \Lambda,\ i_x = 1, 2, ..., N,\ j_{x,\alpha} = 1, 2 \\ 0 & \text{otherwise} \end{cases}.$$

Thus the integral vanishes if the product is incomplete with respect to the lattice, the degenerate states α or σ. Finally, we must impose periodic boundary conditions in the t-direction. It is evident that we can introduce analytic functions of the nilpotent field. Therefore, we may write for the partition function of the hard-core Bose gas

$$Z_{HC} = \int_{HC} \exp\Big[\sum_{x,x'} \sum_{\alpha,\alpha'=1}^{N} (\delta_{x,x'}\delta_{\alpha,\alpha'} + \frac{\zeta}{N}w_{x,x'})\eta_x^{\alpha,1}\eta_{x'}^{\alpha',2} \Big].$$

The nilpotent field $\eta_x^{\alpha,\sigma}$ is closely related to a Grassmann field: the algebra, generated by $\{\eta_x^{\alpha,\sigma}\}$, can be constructed from anticommuting Grassmann variables[13] $\{\psi_x^{\alpha,\sigma}, \bar{\psi}_x^{\alpha,\sigma}\}$ as

$$\eta_x^{\alpha,\sigma} = (-1)^{\sigma}\psi_x^{\alpha,\sigma}\bar{\psi}_x^{\alpha,\sigma}.$$

Using the usual Grassmann integral[13], the partition function now reads

$$Z_{HC} =$$

$$\int \exp\Big[\sum_{x,x'} \sum_{\alpha,\alpha'=1}^{N} (\delta_{x,x'}\delta_{\alpha,\alpha'} + \frac{\zeta}{N}w_{x,x'})\psi_x^{\alpha,1}\bar{\psi}_x^{\alpha,1}\bar{\psi}_{x'}^{\alpha',2}\psi_{x'}^{\alpha',2} \Big] \prod d\psi_x^{\alpha,\sigma} d\bar{\psi}_x^{\alpha,\sigma}.$$

$$(10)$$

Here we notice an identity for the diagonal term:

$$\exp(\psi_x^{\alpha,1}\bar{\psi}_x^{\alpha,1}\bar{\psi}_x^{\alpha,2}\psi_x^{\alpha,2}) = 1 + \psi_x^{\alpha,1}\bar{\psi}_x^{\alpha,1}\bar{\psi}_x^{\alpha,2}\psi_x^{\alpha,2}$$

$$= \exp[(\psi_x^{\alpha,1}\psi_x^{\alpha,2} + \bar{\psi}_x^{\alpha,1}\bar{\psi}_x^{\alpha,2})] - (\psi_x^{\alpha,1}\psi_x^{\alpha,2} + \bar{\psi}_x^{\alpha,1}\bar{\psi}_x^{\alpha,2}).$$

The second term on the r.h.s. does not contribute to the partition function, since there can only be a factor $u_{r,r'}\psi_{t,r}^{\alpha,1}\bar{\psi}_{t,r}^{\alpha,1}$ or $u_{r',r}\bar{\psi}_{t,r}^{\alpha,2}\psi_{t,r}^{\alpha,2}$ from the bosons in (10). Thus, the diagonal term in Z_{HC} can be replaced by a term that is only bilinear in the Grassmann field. The w–dependent term in Z_{HC}, which describes the bosons, can also be expressed bilinearly in the Grassmann field when we introduce two complex Gaussian fields ("Hubbard– Stratonovich transformation"). Two fields are required here, since w is not a positive matrix. However, we obtain a positive matrix v_s when we add a positive diagonal matrix to w as

$$w_{x,x'} = w_{x,x'} + (s-s)\delta_{x,x'} =: (v_s)_{x,x'} - s\delta_{x,x'},$$

with a sufficiently large s. (Physical results should not depend on s. This will be confirmed in the results of the limit $N \to \infty$ below.) With

$$\rho_x = \sum_\alpha \psi_x^{\alpha,1}\bar{\psi}_x^{\alpha,1}, \quad \bar{\rho}_x = \sum_\alpha \bar{\psi}_x^{\alpha,2}\psi_x^{\alpha,2}$$

we obtain the identity

$$\left(\frac{\pi\zeta^2}{sN^2}\right)^{\beta\mathcal{N}} \exp[\frac{\zeta}{N}(\rho, w\bar{\rho})] =$$

$$\int \exp\left[-\frac{N}{\zeta}(\varphi, v_s^{-1}\bar{\varphi}) - \frac{N}{s\zeta}(\chi, \bar{\chi}) + (\rho, \varphi) + (\varphi, \bar{\rho}) + i(\rho, \bar{\chi}) + i(\chi, \bar{\rho})\right] \prod d\varphi_x d\chi_x,$$

(11)

where the scalar product means $(\varphi, v_s^{-1}\bar{\varphi}) = \sum_{x,x'} \varphi_x v_{s;x,x'}^{-1}\bar{\varphi}_{x'}$. The r.h.s. of (11) can be substituted into Z_{HC}, and the bilinear Grassmann term can be integrated. This leads to

$$Z_{HC} = \left(\frac{\pi\zeta^2}{sN^2}\right)^{-\beta\mathcal{N}} \int \exp\left\{-N\left[\frac{1}{\zeta}(\varphi, v_s^{-1}\bar{\varphi}) + \frac{1}{s\zeta}(\chi, \bar{\chi})\right.\right.$$
$$\left.\left. - \sum_x \log[1 + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)]\right]\right\} \prod d\varphi_x d\chi_x.$$
(12)

It should be noticed that the field χ can also be integrated out in principle. However, this is difficult if $N \gg 1$.

We notice that the expression in the exponent is invariant under a global phase transformation of the complex field: $\varphi, \chi \to e^{i\kappa}\varphi, e^{i\kappa}\chi$ and $\bar{\varphi}, \bar{\chi} \to e^{-i\kappa}\bar{\varphi}, e^{-i\kappa}\bar{\chi}$. Furthermore, the logarithmic term of the action is also symmetric under a local $U(1)$-transformation. This means that the dependence of the logarithmic term on the local phase of φ_x can be gauged away, and this term depends only on the modulus of φ_x. We will see in Sect. 5 that

the symmetry under this phase transformation is spontaneously broken. As a consequence, there is a one-component Goldstone mode.

The total density of bosons can be expressed within the new effective complex fields φ and χ. From Eq. (9) we obtain

$$n = \frac{\zeta}{N\mathcal{N}\beta}\frac{\partial}{\partial\zeta}\log Z_{HC} = \frac{1}{\zeta\mathcal{N}\beta}\Big[\langle(\varphi, v_s^{-1}\bar{\varphi})\rangle + \frac{1}{s}\langle(\chi,\bar{\chi})\rangle\Big] + \frac{2}{N}, \qquad (13)$$

where

$$
\begin{aligned}
\langle\ldots\rangle &= \Big(\frac{\pi\zeta^2}{sN^2}\Big)^{-\beta\mathcal{N}}\frac{1}{Z_{HC}}\int\ldots\exp\Big\{-N\Big[\frac{1}{\zeta}(\varphi, v_s^{-1}\bar{\varphi}) + \frac{1}{s\zeta}(\chi,\bar{\chi})\\
&\quad - \sum_x\log[1 + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)]\Big]\Big\}\prod d\varphi_x d\chi_x.
\end{aligned}
\qquad (14)
$$

3. $N \to \infty$: CLASSICAL-FIELD EQUATIONS

The action in (12) depends on the number of states only through the prefactor N. This suggests that a saddle-point integration can be performed for Z_{HC}. For this purpose it is convenient to rescale the fields first:

$$\varphi \to \zeta^{-1/2}\varphi, \quad \chi \to \zeta^{-1/2}\chi.$$

We will use the same name for the rescaled fields. Then the saddle-point equations read

$$\frac{\partial S}{\partial\varphi_x} = \sum_{x'}(v_s^{-1})_{x,x'}\bar{\varphi}_{x'} - \frac{\bar{\varphi}_x + i\bar{\chi}_x}{\zeta^{-1} + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)} = 0 \qquad (15)$$

$$\frac{\partial S}{\partial\bar{\varphi}_x} = \sum_{x'}(v_s^{-1})_{x',x}\varphi_{x'} - \frac{\varphi_x + i\chi_x}{\zeta^{-1} + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)} = 0 \qquad (16)$$

$$\frac{\partial S}{\partial\chi_x} = \frac{1}{s}\bar{\chi}_x - \frac{i(\bar{\varphi}_x + i\bar{\chi}_x)}{\zeta^{-1} + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)} = 0 \qquad (17)$$

$$\frac{\partial S}{\partial\bar{\chi}_x} = \frac{1}{s}\chi_x - \frac{i(\varphi_x + i\chi_x)}{\zeta^{-1} + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)} = 0 \qquad (18)$$

Eqs. (15) - (18) correspond to a discrete version of the Gross-Pitaevskii (or non-linear Schrödinger) equation, often used for the description of a weakly-interacting Bose gas[7,8], a case in which we can assume that fields are small. Expansion in terms of the fields yields an equation for φ:

$$\sum_{x'}(v_s)_{x',x}^{-1}\varphi_{x'} + \Big[-\frac{1}{s+z} + \frac{z^2}{(s+z)^4}\varphi_x\bar{\varphi}_x\Big]\varphi_x \sim 0.$$

In general, it is not possible to solve these equations. Therefore, the assumption of a uniform solution is useful. This is known as the Thomas-Fermi approximation[8].

3.1.   The Thomas-Fermi Approximation

For a uniform solution we obtain with $\sum_{x'}(v_s^{-1})_{x,x'} = 1/(1+s)$ and Eqs. (15)-(18)

$$i\chi = -\frac{s}{1+s}\varphi, \quad i\bar{\chi} = -\frac{s}{1+s}\bar{\varphi}.$$

There is always a trivial solution $\varphi_0 = \bar{\varphi}_0 = \chi_0 = \bar{\chi}_0 = 0$ and a non–trivial solution with

$$\varphi_1\bar{\varphi}_1 = (1+s)^2(1-z).$$

The fugacity ζ has been replaced here by the inverse fugacity $z = \zeta^{-1}$. The saddle-point contribution from the trivial solution gives for the partition function $Z_0 = 1$. Any non–trivial solution breaks the symmetry under phase transformation for $z \neq 1$. The saddle-point equations, however, are invariant under the symmetry transformation because the phase factor is not determined by them. This leads to massless fluctuations that generate long-range correlations. The $N \to \infty$ limit of the partition function is not affected by these fluctuations

$$Z_1 = z^{-N\mathcal{N}\beta}e^{(z-1)N\mathcal{N}\beta}.$$

Since the free energy $-\log Z_{HC}$ must be minimal, the non–trivial saddle point with $Z_{HC} = Z_1$ is valid for $z < 1$ whereas the trivial saddle-point solution with $Z_{HC} = Z_0$ is valid for $z > 1$. This implies for the density of bosons of Eq. (13) in the limit $N \to \infty$

$$n(z) \to \begin{cases} 1-z & \text{for } z < 1 \\ 0 & \text{for } z > 1 \end{cases}.$$

Thus $z = 1$ is the critical point. According to the definition of z as the inverse fugacity of the bosons, $z = 1$ separates the condensed phase ($z < 1$) from the normal-fluid phase ($z > 1$). Corrections of $o(N^{-1})$ to $n(z)$ will be evaluated in Sect. 5.1.

4. $1/N$-CORRECTIONS: QUASIPARTICLES

In order to investigate the stability of the saddle-point solutions against fluctuations, we shall consider now

$$\varphi \approx \varphi_1 + \delta\varphi' + i\delta\varphi'', \quad \chi \approx \chi_1 + \delta\chi' + i\delta\chi''.$$

With $\delta\phi = (\delta\varphi', \delta\varphi'', \delta\chi', \delta\chi'')$ we obtain for the partition function in Gaussian approximation

$$Z_{HC} \approx Z_\nu \int \exp[-N(\delta\phi, \mathcal{G}_{s,\nu}^{-1}\delta\phi)] \prod_x d\delta\phi_x \tag{19}$$

with the propagator (Green's function) $\mathcal{G}_{s,\nu}$. It remains to evaluate the latter. For this purpose it is necessary to choose a specific $u = e^{-H}$ (or $H = -\log u$), for instance,

$$u_{r,r'} = \begin{cases} J/2d & \text{for } r, r' \text{ nearest neighbors} \\ (1 - J) & \text{for } r' = r \\ 0 & \text{otherwise} \end{cases} \qquad (20)$$

Then the eigenvalues of the matrix w are

$$\tilde{w} = e^{i\omega}[1 - J + \frac{J}{d} \sum_{j=1}^{d} \cos(k_j)] \qquad (21)$$

with Matsubara frequency ω and d-dimensional wavevector components k_j with $-\pi \le \omega, k_j < \pi$. The eigenvalues are bounded by $|\tilde{w}| \le 1$. It is sufficient to consider $s = 1$ to get a positive matrix v_1. Then a simple calculation gives the Green's function

$$\mathcal{G}_{1,\nu}^{-1} \equiv \mathcal{G}_{\nu}^{-1} = \begin{pmatrix} \hat{v}_1^{-1} - A_\nu & -iA_\nu \\ -iA_\nu & 1 + A_\nu \end{pmatrix}$$

with

$$\hat{v}_1^{-1} \sim \frac{1}{2} \begin{pmatrix} 1 + k^2/4\tau & -\omega/2 \\ -\omega/2 & 1 + k^2/4\tau \end{pmatrix}$$

for small wavevectors k and frequencies ω. $\nu = 0, 1$ refers to the two saddle-point solutions within the Thomas-Fermi approximation. The new parameter τ is proportional to the inverse tunneling rate on the d-dimensional lattice: $\tau = d/J$. The 2×2 block matrices depend on the fugacity $1/z$

$$A_0 = \frac{1}{z} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 2z - 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

5. RESULTS

The spectrum of the propagator of the field φ is given as (s. App. A)

$$\epsilon(k) = \sqrt{\frac{\zeta - 1}{\tau} k^2 + (\frac{k^2}{2\tau})^2}. \qquad (22)$$

For a weakly-interacting Boge gas of bosons with mass m there is the well-known Bogoliubov spectrum[15]

$$\epsilon(k) = \sqrt{\mu_0 k^2/m + (k^2/2m)^2}.$$

Since $\mu_0 = \log \zeta$ we can identify our parameter τ with the mass of weakly-interacting bosons. Then Eq. (22) agrees with the Bogoliubov spectrum only for $\zeta \sim 1$, indicating that the dilute limit of the hard-core Bose gas is a weakly-interacting system. The Goldstone mode of $\mathcal{G}_1$ is proportional to

$$\frac{\zeta - 1}{\tau} k^2 - \omega^2.$$

Thus, the sound velocity is $c = \sqrt{(\zeta - 1)/\tau}$. On the other hand, Popov[15] finds $c = \sqrt{\mu_0/m}$. Therefore, the sound velocity of the N state hard-core Bose gas agrees with that of the weakly-interacting bosons only for $\zeta \sim 1$.

5.1. Total Density of Bosons

From Eq. (13) we obtain the expression

$$n = (1 - z)\Theta(1 - z) + n_1/N + o(N^{-2}) \tag{23}$$

with

$$n_1 = 2 + \frac{1}{\beta \mathcal{N}} \mathrm{Tr}(\mathcal{G}_\nu \frac{\partial}{\partial \zeta} \mathcal{G}_\nu^{-1}).$$

Here $\Theta(x)$ is the Heaviside step function. This result indicates that there are no bosons at $z > 1$ in the limit $N \to \infty$, as in the non-interacting Bose gas. However, the density increases linearly for $z < 1$, a regime that is not accessible for the non-interacting Bose gas. For a finite number of states N there is a non-vanishing density of particles for any value of the inverse fugacity z.

5.2. Density of the Condensate

The condensate can be studied by considering the correlation function of the hard-core Bose field

$$C_{x,x'} = \frac{1}{N^2} \sum_{\alpha, \alpha' = 1}^{N} \langle \eta_x^{\alpha,1} \eta_{x'}^{\alpha,2} \rangle.$$

On large scales this does not decay in the condensed phase but exhibits off-diagonal long range order:

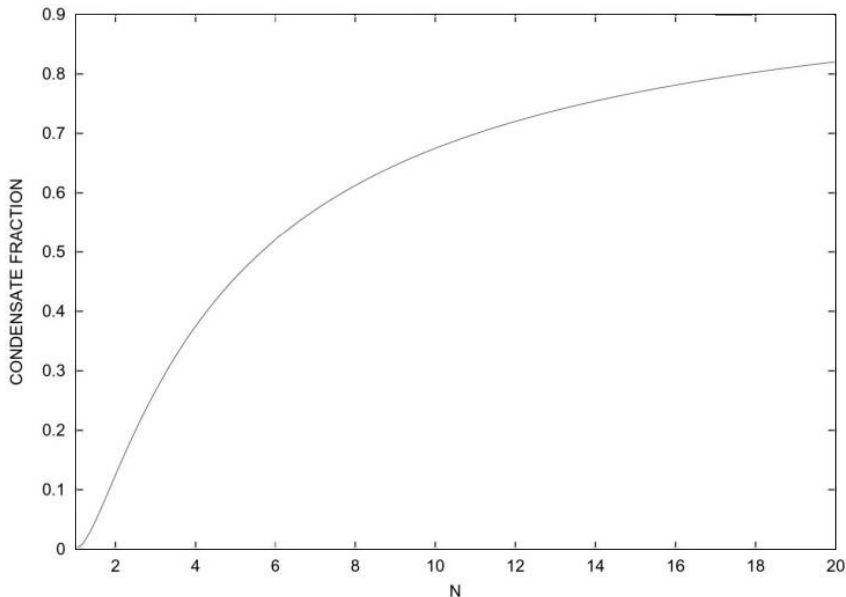$$C_{x,x'} \sim n_0 \quad (|r - r'| \sim \infty),$$

Fig. 1. Fraction of the condensate n_0/n as a function of the number of degenerate states N per site at fugacity $\zeta = 2$ (from Eq. (25)).

where n_0 is the density of the condensate. Using the notation of Sect. 2 we can also express the correlation function of the Bose field as

$$C_{x,x'} = \frac{1}{N^2} \langle \rho_x \bar{\rho}_{x'} \rangle.$$

Eventually, in terms of the fields φ and χ the latter reads

$$C_{x,x'} = -\frac{1}{N}(v_s^{-1})_{x',x} +$$

$$\left\langle \left[\varphi'_x - \frac{1}{N}\frac{\varphi_x + i\chi_x}{z + (\varphi_x + i\chi_x)(\bar{\varphi}_x + i\bar{\chi}_x)}\right]\left[\bar{\varphi}'_{x'} - \frac{1}{N}\frac{\bar{\varphi}_{x'} + i\bar{\chi}_{x'}}{z + (\varphi_{x'} + i\chi_{x'})(\bar{\varphi}_{x'} + i\bar{\chi}_{x'})}\right]\right\rangle$$

with $\varphi'_x = \sum_{x'}(v_s^{-1})_{x,x'}\varphi_{x'}$. Using the result of the saddle-point integration this expression leads for $|r - r'| \to \infty$ to

$$n_0 = (1 - \frac{1}{N})^2(1 - z)\Theta(1 - z) \tag{24}$$

for the density of the condensate. The prefactor $(1 - 1/N)^2$ indicates a suppression of the condensate due to increasing interaction with a decreasing

number of particles states N at each lattice site. In Eq. (24) terms of higher order in $1/N$ are neglected. It is expected that they lead to additional terms such that n_0 does not vanish at $N = 1$. Combining (23) and (24) the condensate fraction reads

$$\frac{n_0}{n} = (1 - \frac{1}{N})^2 \frac{(1 - z)}{1 - z + n_1/N}\Theta(1 - z) \qquad (25)$$

which is plotted in Fig.1.

6. CONCLUSIONS

A hard-core Bose gas on a lattice has been used to study the effect of interaction in an optical lattice. Introducing N degenerate states at each lattice site and a hard-core interaction only between the same state, the limit $N \to \infty$ can be solved by a saddle-point integration. This limit exhibits a transition from a normal state to a Bose-Einstein condensate if the fugacity $\zeta = 1$. The limit $N \to \infty$ is very special, since the total density of bosons vanishes for $\zeta < 1$. However, $1/N$-corrections lead to a non-vanishing density of bosons for any value of ζ. On the other hand, $1/N$-corrections indicate a depletion of the condensate ($\zeta > 1$). These results agree with the observation that the condensate fraction decreases with an increasing coupling constant in the Bose-Hubbard model[5]. Further studies are neccessary in order to find the effect of very strong interaction when $N \sim 1$.

APPENDIX A: EFFECTIVE PROPAGATOR FOR THE FIELD φ

Starting from the partition function Z_{HC} of Eq. (19), the field χ can be integrated out. The result is an effective propagator of the field φ

$$\mathcal{G}_\nu = (v_1^{-1} - A_\nu + B_\nu)^{-1},$$

where we have

$$B_0 = \frac{1}{z(1+z)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad B_1 = \frac{1}{2}\begin{pmatrix} (2z-1)^2/z & 0 \\ 0 & 1 \end{pmatrix}.$$

Then a straightforward calculation gives the following expressions

$$\mathcal{G}_0^{-1} \sim \frac{1}{2} \begin{pmatrix} (z-1)/(z+1) + k^2/4\tau & -\omega/2 \\ -\omega/2 & (z-1)/(z+1) + k^2/4\tau \end{pmatrix}$$

and

$$\mathcal{G}_1^{-1} \sim \frac{1}{2} \begin{pmatrix} (1-z)/z + k^2/4\tau & -\omega/2 \\ -\omega/2 & k^2/4\tau \end{pmatrix}.$$

From $\mathcal{G}_1^{-1}$ we obtain for the spectrum of the condensed phase (i.e. $z < 1$) the expression

$$\epsilon(k) = \sqrt{\frac{(1-z)}{z}\frac{k^2}{\tau} + (\frac{k^2}{2\tau})^2}.$$

REFERENCES

1. M.H. Anderson et al., Science **269**, 198 (1995); C.C. Bradley et al., Phys. Rev. Lett. **75**, 1687 (1995); K.B. Davis et al., Phys. Rev. Lett **75**, 3969 (1995).
2. R. Feynman, *Statistical Physics* (Benjamin, Reading, 1972).
3. K. Huang, in *Studies in Statistical Mechanics* (North-Holland, Amsterdam, 1969).
4. D. Jaksch et al., *Phys. Rev. Lett.* **81**, 3108 (1998).
5. D. van Oosten, P. van Straten, and H.T.C. Stoof, *Phys. Rev. A* **63**, 053601 (2001).
6. M.L. Chiofalo, S. Succi, and M.P. Tosi, *Phys. Rev. A* **63**, 063613 (2001).
7. V.L. Ginzburg and L.P. Pitaevskii, *Zh. Eksp. Teor. Fiz.* **34**, 1240 (1958) [*Sov. Phys. JETP* **7**, 858 (1958)]; E.P. Gross, *J. Math. Phys. (N.Y.)* **4**, 195 (1963).
8. G. Baym and C. Pethick, *Phys. Rev. Lett.* **76**, 6 (1996); F. Dalfovo and S. Stringari, *Phys. Rev. A* **53**, 2477 (1996); A.L. Fetter, *Phys. Rev. A* **53**, 4245 (1996).
9. Ph. Courteille et al., *Phys. Rev. Lett.* **81**, 69 (1998).
10. J.L. Roberts et al., *Phys. Rev. Lett.* **81**, 5109 (1998).
11. S.L. Cornish et al., *Phys. Rev. Lett.* **85**, 1795 (2000).
12. K. Ziegler, *Physica A* **208**, 177 (1994).
13. J. W. Negele and H. Orland, *Quantum Many - Particle Systems* (Addison - Wesley, New York, 1988).
14. J. Glimm and A. Jaffe, *Quantum Physics* (Springer, New York, 1987).
15. V.N. Popov, *Functional Integrals in Quantum Field Theory and Statistical Physics* (Reidel, Dordrecht, 1983).