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Bose-Einstein condensation in a lattice model

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Abstract

A model of a boson lattice gas is considered with infinite-range hopping and a repulsive single-site potential. It is found that there is a range of critical coupling strengths $\lambda_{c1} < \lambda_{c2} < \lambda_{c3} < \dots$ in this model. For coupling strengths between $\lambda_{c,k}$ and $\lambda_{c,k+1}$, Bose-Einstein condensation is suppressed at densities near the integer values $\rho = 1, \dots, k$. This phenomenon manifests itself also in the pressure-volume diagram at high pressures. It is suggested that this phenomenon persists for finite-range hopping and might be experimentally observable.

1 The model and an expression for the pressure

We consider a model of bosons hopping on a lattice with sites labelled $x = 1, 2, \ldots, V$, given by the hamiltonian

$$H_V = \frac{1}{2V} \sum_{x,y=1}^{V} (a_x^* - a_y^*)(a_x - a_y) + \lambda \sum_{x=1}^{V} n_x(n_x - 1), \tag{1.1}$$

where a_x and a_x^* are annihilation and creation operators satisfying the usual commutation relations $[a_x, a_y^*] = \delta_{x,y}$ and $n_x = a_x^* a_x$. The first term is a mean-field version of the kinetic energy operator; the second term describes a repulsion if $\lambda > 0$, as it discourages more than one particle per site. A similar, but less general model was introduced by Toth [1]. His model is a special case of (1.1) where $\lambda = +\infty$, i.e. there is complete single-site exclusion. A disordered version of Toth's model was considered by Ma et al. [2] and the corresponding model with short-range hopping was analysed using path-integral Monte-Carlo methods by Krauth et al. [3]. A nice introduction to the mathematical analysis of the short-range hopping version of (1.1) is [4].

The grand canonical partition function corresponding to (1.1) is given by

$$Z_V = \sum_{n=0}^{\infty} e^{\beta\mu n} \mathrm{Trace}\, e^{-\beta H_V}, \tag{1.2}$$

where β is the inverse temperature. The pressure $p(\beta, \mu) = \lim_{V\to\infty} \frac{1}{\beta V} \ln Z_V$ in the thermodynamic limit can be expressed as a variational formula using a formalism developed by N. N. Bogoliubov Jr. [5, 6] (see also [7]) and first applied to the boson gas by Ginibre [8]. (For an interesting recent application to a Bose gas model, see [9] and [10].) The result is:

$$\begin{aligned} p(\beta, \mu) &= \sup_{r \geq 0} \Big\{ -r^2 \\ &\quad + \frac{1}{\beta} \ln \mathrm{Trace}\, \exp\left[\beta((\mu - 1)n - \lambda n(n-1) + r(a^* + a))\right] \Big\}. \end{aligned} \tag{1.3}$$

Here the trace is over the representation space of a single oscillator with creation and annihilation operators a^* and a, and number operator $n = a^* a$. Even though this expression for the pressure is exact, the trace still has to be evaluated numerically. The derivation of this formula will be published elsewhere [11]. Here we consider its implications for Bose-Einstein condensation. Bose-Einstein condensation (BEC) occurs in this model if the maximizer $r > 0$, and in that case the density of the condensate is given by $\rho_0 = r^2$. To see this, notice that the kinetic energy term in the Hamiltonian can be diagonalized by means of any orthogonal matrix $O_{k,x}$ satisfying $O_{0,x} = 1/\sqrt{V}$. Defining $c_k^{\#} = \sum_x O_{k,x} a_x^{\#}$ $(k = 0, 1, \ldots, V-1)$ we have

$$\frac{1}{2V} \sum_{x,y} (a_x^* - a_y^*)(a_x - a_y) = \sum_{k=1}^{V-1} c_k^* c_k. \tag{1.4}$$

Replacing this term by $\alpha c_0^* c_0 + \sum_{k=1}^{V-1} c_k^* c_k$ there is an analogous formula for the pressure:

$$\begin{aligned} p(\beta, \mu, \alpha) \;=\; & \sup_{r \geq 0} \Big\{ -\frac{r^2}{1-\alpha} \\ & + \frac{1}{\beta} \ln \mathrm{Trace} \exp \left[\beta((\mu - 1)n - \lambda n(n-1) + r(a^* + a)) \right] \Big\}. \end{aligned} \tag{1.5}$$

Now, the density of the condensate is given by

$$\rho_0 = \lim_{V \to \infty} \frac{1}{V} \langle c_0^* c_0 \rangle = -\frac{dp}{d\alpha}\bigg|_{\alpha=0} = r^2. \tag{1.6}$$

This trick for obtaining ρ_0 of introducing a gap in the spectrum of the kinetic term, is quite standard; see for example [12] and [13].

2 Analysis of the phase diagram

The phase diagram is determined by the maximization problem (1.3). To find the maximizer we differentiate to get

$$2r = \langle a + a^* \rangle = \frac{\mathrm{Trace}(a + a^*) \exp \left[\beta((\mu - 1)n - \lambda n(n-1) + r(a^* + a)) \right]}{\mathrm{Trace} \exp \left[\beta((\mu - 1)n - \lambda n(n-1) + r(a^* + a)) \right]}. \tag{2.1}$$

It is convenient to define

$$\tilde{p}(r) = \frac{1}{\beta} \ln \mathrm{Trace} \exp \left[\beta((\mu - 1)n - \lambda n(n-1) + r(a^* + a)) \right] \tag{2.2}$$

so that (2.1) reads $2r = \tilde{p}'(r)$. Differentiating once more we have

$$\tilde{p}''(r) = \beta\,(A - \langle A\rangle \mid A - \langle A\rangle)_{H(r)}, \tag{2.3}$$

where $A = a^* + a$ and $(\cdot|\cdot)_H$ denotes the Bogoliubov scalar product:

$$(A \mid B)_H = \frac{1}{\beta Z}\int_0^\beta \text{Trace}\,\left[A^* e^{-(\beta-\tau)H} B e^{-\tau H}\right] d\tau, \tag{2.4}$$

with $Z = \text{Trace}\, e^{-\beta H}$ and $H = H(r) = (1-\lambda)\,n + \lambda\,n^2 - r(a+a^*) - \mu\,n$. It follows that $\tilde{p}''(r) \geq 0$ for all $r \geq 0$ so that $\tilde{p}'$ is increasing. In fact, graphs of $\tilde{p}'$ suggest that it is also concave. In fact, a very general conjecture by Bessis et al.[14] suggests that the derivatives should have alternating signs. Some special cases of this conjecture have been proved by Fannes and Werner[15]. Assuming the concavity of $\tilde{p}'(r)$, the maximum in (1.3) must either be attained at $r = 0$ or at a unique $r > 0$. The latter case applies when $\tilde{p}''(0) > 2$. But, $\tilde{p}''(0)$ can be computed exactly as $H(0)$ is diagonal: $H(0) = h_0(n) = -(\mu + \lambda - 1)\,n + \lambda\,n^2$. The denominator in (2.4) is

$$Z_0 = \sum_{n=0}^{\infty} e^{-\beta h_0(n)} = \sum_{n=0}^{\infty} e^{\beta[(\mu+\lambda-1)n - \lambda n^2]}. \tag{2.5}$$

To compute the numerator, remark that

$$\begin{aligned}&\text{Trace}\,\left[(a+a^*)e^{-(\beta-\tau)h_0(n)}(a+a^*)e^{-\tau h_0(n)}\right]\\ &= \sum_{n=1}^{\infty}\left\{e^{-\tau h_0(n)} n e^{-(\beta-\tau)h_0(n-1)} + e^{-(\beta-\tau)h_0(n)} n e^{-\tau h_0(n-1)}\right\}.\end{aligned} \tag{2.6}$$

We therefore compute

$$\int_0^\beta e^{-\tau h_0(n)} e^{-(\beta-\tau)h_0(n-1)} d\tau = \frac{e^{-\beta h_0(n)} - e^{-\beta h_0(n-1)}}{h_0(n-1) - h_0(n)}. \tag{2.7}$$

It follows that

$$\tilde{p}''(0) = \frac{2}{Z_0}\sum_{n=1}^{\infty} n \frac{e^{-\beta h_0(n)} - e^{-\beta h_0(n-1)}}{h_0(n-1) - h_0(n)}. \tag{2.8}$$

Solving the equation $\tilde{p}''(0) = 2$ yields the critical inverse temperature $\beta_c(\mu,\lambda)$. A careful asymptotic analysis shows that the asymptotic behaviour for small μ is given by

$$\beta_c \approx \ln\frac{4}{\lambda}(2\lambda+1)\mu \qquad (\mu \ll \lambda) \tag{2.9}$$

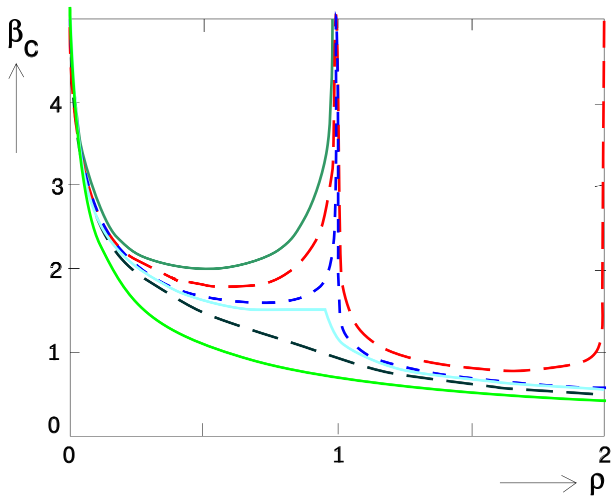

Figure 1: *The critical inverse temperature for a number of values of λ. The lower curve (light green) is for the free lattice gas: $\lambda = 0$, the top curve (dark green) is for the case of complete single-site exclusion $\lambda = +\infty$. Intermediate values are: $\lambda = 2$ (black), 2.7 (light blue) , 3 (royal blue) and 5 (red).*

and for large μ by

$$\beta_c \approx \frac{2}{\lambda}\mu \qquad (\mu \gg \lambda). \tag{2.10}$$

For small λ, $\beta_c(\mu, \lambda)$ is simply an interpolation between these asymptotic graphs, but for larger values of λ it diverges in certain intervals of μ. This can be understood as follows. We write the equation $\tilde{p}''(0) = 2$ in the form $\Delta f(\beta, \mu, \lambda) = 0$ where

$$\Delta f(\beta, \mu, \lambda) = 1 + \frac{1}{\mu - 1} + \sum_{n=1}^{\infty} e^{-\beta h(n)} \left\{ 1 - \frac{n}{\Delta h(n)} + \frac{n+1}{\Delta h(n+1)} \right\} \tag{2.11}$$

and $\Delta h(n) = h(n-1) - h(n) = \mu - 1 - 2\lambda(n-1)$. Working out the factor in brackets yields

$$\Delta f(\beta, \mu, \lambda) = 1 + \frac{1}{\mu - 1} + \sum_{n=1}^{\infty} e^{-\beta h(n)} \frac{(2\lambda n - \lambda - \mu + 1)^2 + \mu - (\lambda - 1)^2}{(\mu - 1 - 2\lambda n)(\mu - 1 - 2\lambda(n-1))}. \tag{2.12}$$

For $1 < \mu < 1 + 2\lambda$ the first exponential term dominates. The corresponding factor is only negative if μ is not in the interval between μ_- and μ_+ given by

$$\mu_\pm = \lambda + \frac{1}{2} \pm \frac{1}{2}\sqrt{4\lambda^2 - 12\lambda + 1}. \tag{2.13}$$

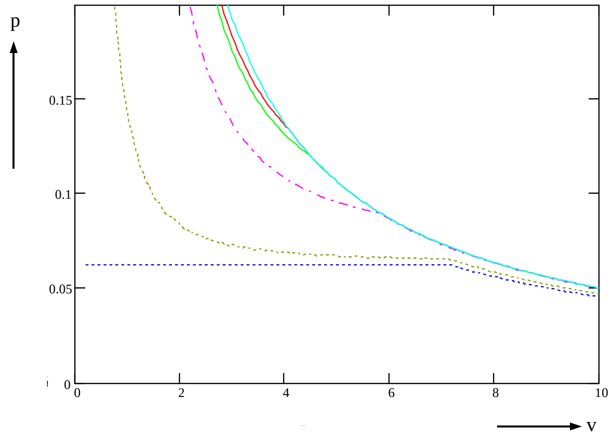

Figure 2: *The pressure vs. volume diagram for* $\beta = 2.5$ *and* $\lambda = 0.1, 3, 5$ *and* $+\infty$.

Of course, this can only happen if $4\lambda^2 - 12\lambda + 1 \geq 0$, i.e. if

$$\lambda \geq \lambda_1 = \frac{1}{2}(3 + \sqrt{8}). \tag{2.14}$$

Similarly, for $1 + 2(k-1)\lambda < \mu < 1 + 2k\lambda$ one finds a gap in the interval $[\mu_{k,-}, \mu_{k,+}]$ given by

$$\mu_{k,\pm} = (2k-1)\lambda + \frac{1}{2} \pm \sqrt{\lambda^2 - (2k+1)\lambda + \frac{1}{4}} \tag{2.15}$$

which can happen only if

$$\lambda \geq \lambda_k = k + \frac{1}{2} + \sqrt{k(k+1)}. \tag{2.16}$$

If μ approaches $\mu_\pm$ from outside the forbidden interval, the critical inverse temperature β_c diverges.

To compute the inverse critical temperature as a function of the density we must solve implicitly the equation

$$\rho = \frac{\partial p}{\partial \mu} = \frac{\sum_{n=1}^{\infty} n \, e^{\beta[(\mu+\lambda-1)n - \lambda n^2]}}{\sum_{n=0}^{\infty} e^{\beta[(\mu+\lambda-1)n - \lambda n^2]}} \tag{2.17}$$

with $\beta = \beta_c(\mu)$. The gaps in μ do not mean that there are gaps in the density. The reason is that for non-integer values of ρ, the curves $\beta(\mu)$ defined implicitly by (2.17) have asymptotes at $\mu = 2(k-1)\lambda + 1$. Indeed, for large β the function $\rho(\beta, \mu)$ tends to a step function: $\rho(\beta, \mu) \sim 0$ if $\mu < 1$ and $\rho(\beta, \mu) \sim k$ if $2(k-1)\lambda < \mu < 2k\lambda + 1$. Numerical solution of the implicit equations (2.17) and $\tilde{p}''(0) = 2$ yields the phase diagram of Figure 1.

We also compute the pressure p as a function of the density. For this, one needs to approximate the trace in (2.2) in case $\beta > \beta_c$ (otherwise the trace is a simple sum which can be easily truncated). This can be done using the Trotter product formula, where, for greater accuracy, we use the formula

$$\langle n \,|\, e^{r(a+a^*)} \,|\, m \rangle = \sqrt{n!m!} \sum_{k=0}^{n \wedge m} \frac{r^{n+m-2k}}{k!(n-k)!(m-k)!} e^{r^2/2}. \tag{2.18}$$

The resulting graphs, for several values of λ and for $\beta = 2$ are depicted in Figures 2 and 3.

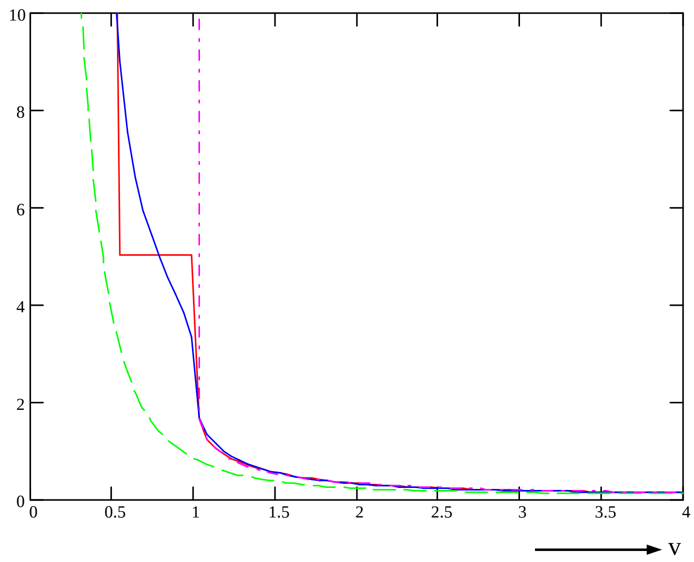

Figure 3: *The pressure vs. volume diagram at higher values of the pressure.*

Figure 2 shows that for small values of λ the pressure is close to that of the free lattice gas except for small values of the specific volume v, where it diverges. There is a clear kink in all the graphs corresponding to the onset of Bose-Einstein condensation. As λ increases, the onset of condensation moves to lower values of v. This point is the right most point of the β_c versus ρ curve of Figure 1 where it intersects with the line $\beta = 2$. For $\lambda > \lambda_1$ we expect another feature in the graph of $p(v)$ at even smaller values of v.

This is visible in Figure 3, but occurs at much higher pressures and cannot, therefore be seen at the scale of Figure 2.

Similarly, at still higher pressures, one observes another s-bend in the graph for lambda-values above λ_2. Interestingly, it seems that the highest-pressure transition is of higher order whereas the lower transitions are first-order:

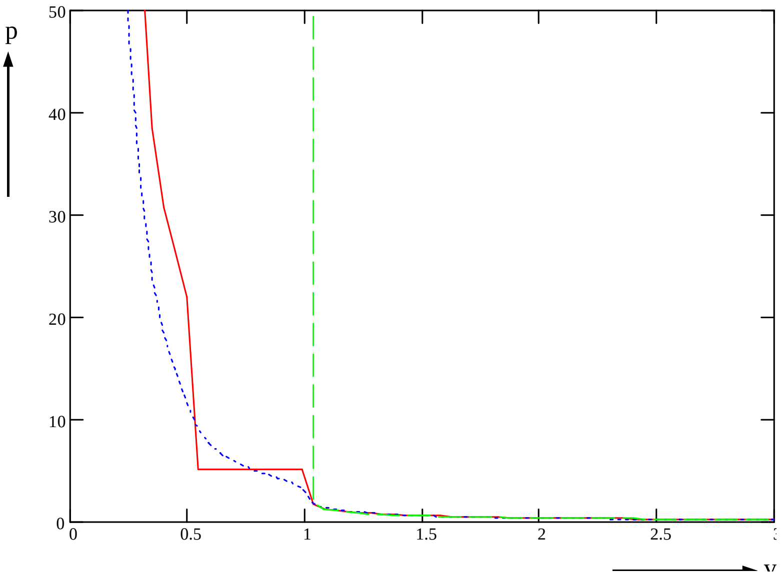

Figure 4: *The pressure vs. volume diagram at still higher values of the pressure.*

The graph of the condensate fraction, i.e. the density of the condensate divided by the total density is also of interest. It is shown in Figure 5. Notice that the condensate at small values of λ is higher than that for the free gas, whereas it is lower for higher values of λ.

Notice also that there is a clear modulation in the condensate fraction. This is not a computational error but is due to the suppression of the condensate at integer densities. A more accurate computation shows this more clearly: see Figure 6.

An intuitive explanation for the suppression of Bose-Einstein condensation at integer values of the density is that at or near these values the particles tend to be evenly distributed over the lattice points and the strong

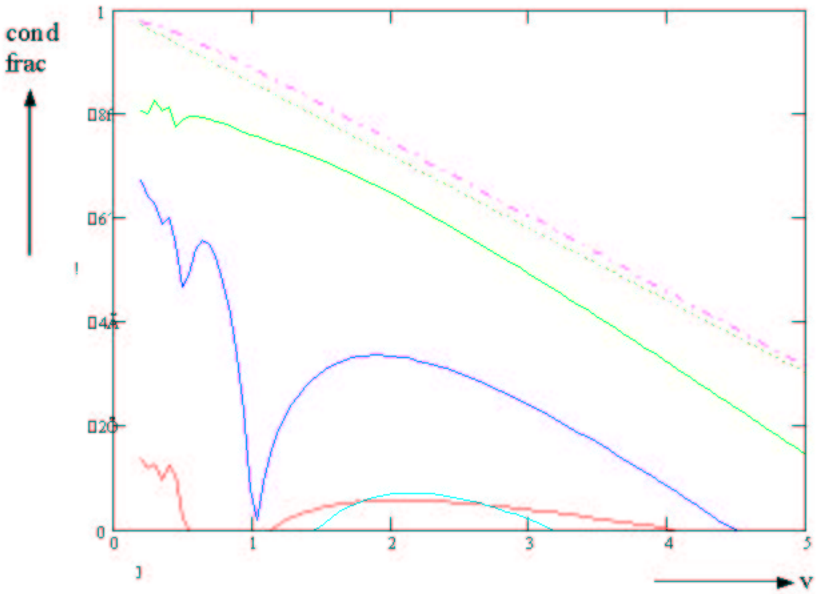

Figure 5: *The condensate fraction as a function of the specific volume for several interaction strengths.*

repulsion tends to restrict their freedom to hop from site to site. The resulting states are almost eigenstates of the number operators n_x and therefore asymptotically almost orthogonal to the ground state of the kinetic energy. This explanation is quite generally valid and we may expect therefore that this phenomenon should occur in general systems of bosons on a lattice with strong repulsion. It would be interesting to find experimental evidence for this phenomenon.

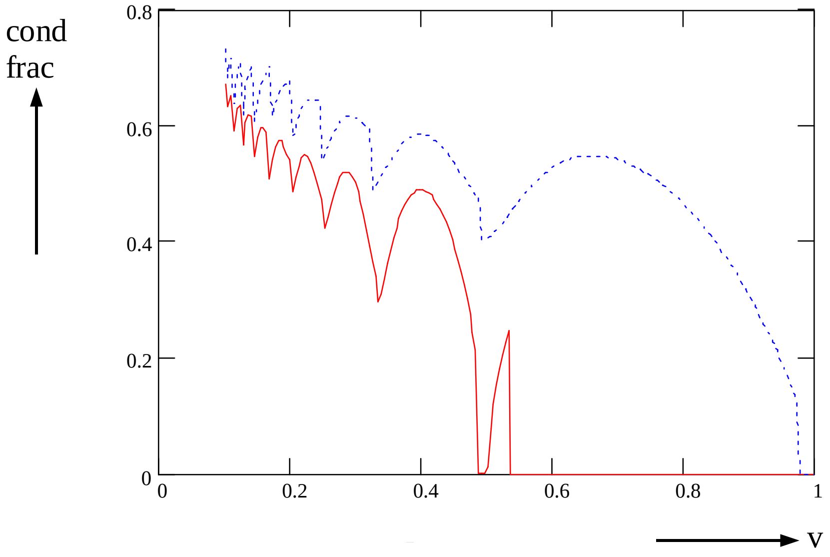

Figure 6: *The condensate fraction for $\lambda = 3$ (dashed blue line) and $\lambda = 5$ (red line).*

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