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Exact Solution of the Infinite-Range-Hopping Bose–Hubbard Model

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The thermodynamic behavior of the Bose–Hubbard model is solved for any temperature and any chemical potential. It is found that there is a range of critical coupling strengths $\lambda_{c1} < \lambda_{c2} < \lambda_{c3} < \cdots$ 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 $\rho = 1,\ldots, k$ with an energy gap. This is known as a Mott insulator phase and was previously shown only for zero temperature. In the context of ultra-cold atoms, this phenomenon was experimentally observed in 2002[(1)] but, in the Bose–Hubbard model, it manifests itself also in the pressure-volume diagram at high pressures. It is suggested that this phenomenon persists for finite-range hopping and might also be experimentally observable.

KEY WORDS: Bose–Hubbard model; Bose condensation; Mott transition.

1. THE INFINITE-RANGE HOPPING BOSE–HUBBARD MODEL

Experimentally, the Mott insulator phase transition has recently been observed[(1)] for a ^{87}Rb Bose condensate in a three-dimensional optical lattice potential. The physical model for this experiment corresponds to the Bose–Hubbard Hamiltonian:

$$H^{\mathrm{BH}} = J \sum_{x,\, y:\, |x-y|=1} (a_x^* - a_y^*)(a_x - a_y) + \frac{U}{2} \sum_x n_x(n_x - 1) + \sum_x \epsilon_x n_x, \tag{1.1}$$

where ϵ_x denotes the energy offset of the x-th lattice site due to the external confinement of the atoms.[(2)] Here a_x and a_x^* are annihilation and creation operators satisfying the usual commutation relations $[a_x, a_y^*] = \delta_{x,y}$ and $n_x = a_x^* a_x$ whereas the Bose model is hopping on a lattice with sites labelled

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$x = 1, 2, \ldots, V$. The first term ($J > 0$) is the kinetic energy operator; the second term describes a repulsion if $\lambda = u/2 > 0$, as it discourages more than one particle per site.

This model was originally introduced by Fisher *et al.*[3] without external potential ϵ. In ref. 3, the authors also analysed the infinite-range hopping version of (1.1) but only for zero-temperature, and their analysis is not exact. The infinite-range hopping model is given by the Hamiltonian

$$H_V = \frac{1}{2V} \sum_{x, y=1}^{V} (a_x^* - a_y^*)(a_x - a_y) + \lambda \sum_{x=1}^{V} n_x(n_x - 1), \tag{1.2}$$

(Cf. also ref. 4.) This Hamiltonian is in fact a mean-field version of (1.1) but in terms of the kinetic energy rather than the interaction. In particular, as in all mean-field models, the lattice structure is irrelevant and there is no dependence on dimensionality.

The model (1.1) and the mean field version (1.2) have been studied before *but mostly for zero-temperature*, see refs. 3–8, using an analysis of the ground state combined with perturbation theory or/and numerical computations. Here we determine the corresponding phase diagram of the infinite-range hopping Bose–Hubbard model (1.2) for *any inverse temperature $\beta > 0$* and *any chemical potential μ*.

A similar, but less general model was introduced by Toth.[9] (This model was also considered by Kirson[10]). His model is a special case of (1.2) where $\lambda = +\infty$, i.e., there is complete single-site exclusion. A disordered version of Toth's model was considered by Ma *et al.*[11] and the corresponding model with short-range hopping was analysed using path-integral Monte-Carlo methods by Krauth *et al.*[12] A nice introduction to the mathematical analysis of the short-range hopping version of (1.2), i.e., (1.1) without the last term, is ref. 13. The first proof of Bose–Einstein condensation in the original nearest-neighbor model (1.1) without external potential ϵ and with $\lambda = +\infty$, was achieved in ref. 24 using reflection positivity.

The grand canonical partition function corresponding to (1.2) is given by

$$Z_V = \sum_{n=0}^{\infty} e^{\beta\mu n} \operatorname{Trace} e^{-\beta H_V}, \tag{1.3}$$

where β is the inverse temperature, and the trace is over the n-particle subspace. 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.[14, 15] (see also refs. 16–18) and applied to the boson gas by Ginibre.[19] (For an interesting recent application to a continuum Bose gas model, see refs. 20 and 21.) This is done in Appendix A and the result is:

$$p(\beta, \mu) = \sup_{r \geqslant 0} \left\{ -r^2 + \frac{1}{\beta} \ln \text{Trace} \exp[\beta((\mu - 1)\, n - \lambda n(n-1) + r(a^* + a))] \right\}. \tag{1.4}$$

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. Here we consider its implications for Bose–Einstein condensation. Bose–Einstein condensation 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 $c_k^\# = \sum_x O_{k,x} a_x^\#$ $(k = 0, 1,..., V-1)$ we have

$$\frac{1}{2V} \sum_{x,y} (a_x^* - a_y^*)(a_x - a_y) = \sum_{k=1}^{V-1} c_k^* c_k. \tag{1.5}$$

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:

$$p(\beta, \mu, \alpha) = \sup_{r \geqslant 0} \left\{ -\frac{r^2}{1-\alpha} + \frac{1}{\beta} \ln \text{Trace} \exp[\beta((\mu - 1)\, n - \lambda n(n-1) + r(a^* + a))] \right\}. \tag{1.6}$$

Now, the density of the condensate is given by

$$\rho_0 = \lim_{V \to \infty} \frac{1}{V} \langle c_0^* c_0 \rangle = -\frac{dp}{d\alpha}\bigg|_{\alpha = 0} = r^2. \tag{1.7}$$

This trick for obtaining ρ_0 of introducing a gap in the spectrum of the kinetic term, is quite standard; see for example refs. 22 and 23.

By numerical computation of the trace in (1.4) we obtain the solution r of the variational problem and find that there is Bose–Einstein condensation at low temperatures for the infinite-range hopping Bose–Hubbard model (1.2). This analysis is performed for arbitrary coupling parameter λ. (The rigorous existence of Bose–Einstein condensation at low enough temperatures in fact only depends on a well-known general conjecture.) We also show that the Bose–Einstein condensation disappears at densities near the integer values $\rho = 1, \ldots, k$ if the coupling parameter λ lies in the range $\lambda_k < \lambda < \lambda_{k+1}$, where the values λ_k can be computed exactly. This specific thermodynamic behavior corresponds to a "Mott insulator phase," where there is an energy gap for all excitations (cf. (2.13) and (2.14)). Our analysis therefore extends the known behaviour of the model to arbitrary temperatures.

2. ANALYSIS OF THE PHASE DIAGRAM

The phase diagram is determined by the maximization problem (1.4). To find the maximizer we differentiate to get

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

It is convenient to define

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

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 $(\cdot \mid \cdot)_H$ denotes the Bogoliubov scalar product (see, e.g., refs. 19 and 25):

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

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 $\tilde{p}''(r) \geqslant 0$ for all $r \geqslant 0$ so that $\tilde{p}'$ is increasing ($\tilde{p}'(0) = 0$). In fact, graphs of $\tilde{p}'$ suggest that it is also concave, see Fig. 1. Indeed, a very general conjecture by Bessis *et al.*[26] suggests that the derivatives should have alternating signs. Some special cases of this conjecture have been proved by Fannes and Werner.[27] Assuming the concavity of $\tilde{p}'(r)$, the maximum in (1.6) must either be attained at $r = 0$ or at a unique $r > 0$.

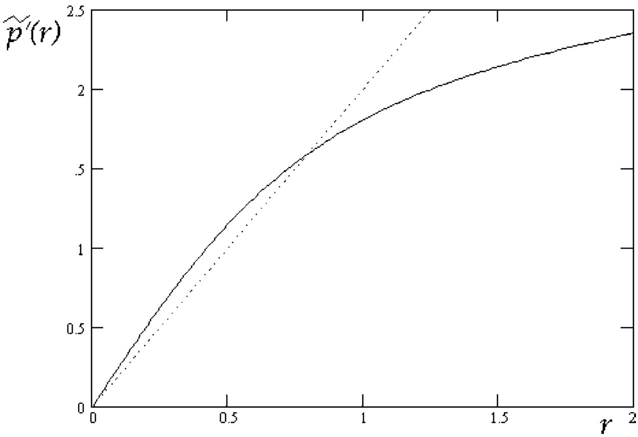

Fig. 1. Illustration of $\tilde{p}'(r)$. The dotted line corresponds to the straight line $2r$ and its intersection with $\tilde{p}'(r)$ gives the solution of the variational problem.

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

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

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 $\beta_c(\mu, \lambda)$. 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

$$\Delta f(\beta,\mu,\lambda)=1+\frac{1}{\mu-1}+\sum_{n=1}^{\infty} e^{-\beta h_0(n)}\left\{1-\frac{n}{\Delta h_0(n)}+\frac{n+1}{\Delta h_0(n+1)}\right\} \tag{2.9}$$

and $\Delta h_0(n)=h_0(n-1)-h_0(n)=\mu-1-2\lambda(n-1)$. Working out the factor in brackets yields

$$\Delta f(\beta,\mu,\lambda)=1+\frac{1}{\mu-1}+\sum_{n=1}^{\infty} e^{-\beta h_0(n)}\frac{(2\lambda n-\lambda-\mu+1)^2+\mu-(\lambda-1)^2}{(\mu-1-2\lambda n)(\mu-1-2\lambda(n-1))}. \tag{2.10}$$

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

$$\mu_\pm=\lambda+\tfrac{1}{2}\pm\tfrac{1}{2}\sqrt{4\lambda^2-12\lambda+1}. \tag{2.11}$$

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

$$\lambda\geqslant\lambda_1=\tfrac{1}{2}(3+\sqrt{8}). \tag{2.12}$$

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

$$\mu_{k,\pm}=(2k-1)\lambda+\tfrac{1}{2}\pm\sqrt{\lambda^2-(2k+1)\lambda+\tfrac{1}{4}} \tag{2.13}$$

which can happen only if

$$\lambda\geqslant\lambda_k=k+\tfrac{1}{2}+\sqrt{k(k+1)}. \tag{2.14}$$

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

$$\rho=\rho(\beta,\mu)=\frac{\partial p}{\partial\mu}=\frac{\sum_{n=1}^{\infty} n e^{\beta[(\mu+\lambda-1)n-\lambda n^2]}}{\sum_{n=0}^{\infty} e^{\beta[(\mu+\lambda-1)n-\lambda n^2]}} \tag{2.15}$$

with $\beta=\beta_c(\mu)$. The gaps in μ do not mean that there are gaps in the density. In fact, for large β the function $\rho(\beta,\mu)$ defined by (2.15) tends to a

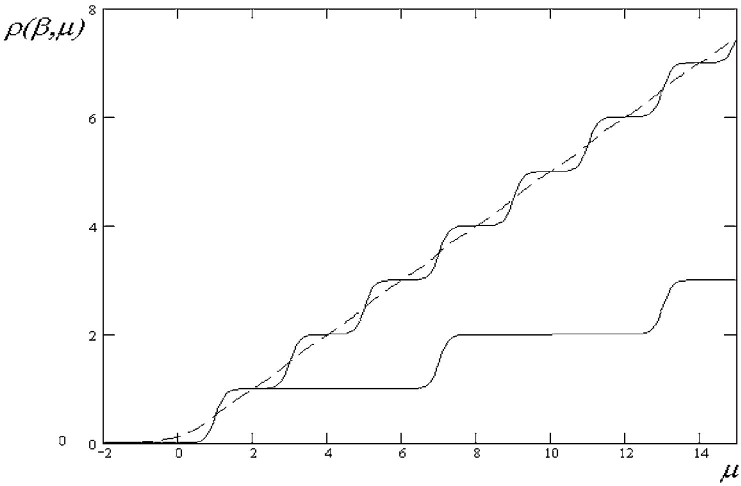

Fig. 2. Illustration of the particle density $\rho(\beta, \mu)$ as a function of μ for different values of β. Notice that, for $\beta \to \infty$, $\rho(\beta, \mu)$ tends to a step function.

step function: $\rho(\beta, \mu) \sim 0$ if $\mu < 1$ and $\rho(\beta, \mu) \sim k$ if $2(k-1)\,\lambda + 1 < \mu < 2k\lambda + 1$, see Fig. 2.

Therefore for *non-integer* values of $\rho \in (k-1, k)$, the corresponding $\mu(\beta, \rho)$, solution of (2.15) for fixed β, is $\mu(\beta, \rho) \sim 2(k-1)\,\lambda + 1$ as $\beta \to \infty$ and so, the curves $\beta(\mu, \rho)$ defined implicitly by (2.15) (μ fixed) have asymptotes at $\mu = 2(k-1)\,\lambda + 1$, i.e.,

$$\lim_{\mu \to 2(k-1)\,\lambda + 1} \beta(\mu, \rho) = +\infty.$$

Since $\mu_{k-1,+} < 2(k-1)\,\lambda + 1 < \mu_{k,-}$, the curves $\beta(\mu, \rho)$ and $\tilde{p}''(0) = 2$ always intersect. This intersection corresponds to the critical inverse temperature $\beta_c(\mu)$. Numerical solution of the implicit equations (2.15) and $\tilde{p}''(0) = 2$ yields the phase diagram of Fig. 3.

It is of interest to analyse the asymptotic behavior for small λ. Assuming that $\beta\lambda \ll 1$ we can replace the terms $e^{-\beta h_0(n)}$ in (2.10) by $e^{n\beta(\mu-1)}$. Using also the approximation

$$-\frac{n}{\Delta h_0(n)} \approx \frac{n}{1-\mu}\left(1 - \frac{2(n-1)\,\lambda}{1-\mu}\right)$$

the series can be summed:

$$\Delta f(\beta, \mu, \lambda) \approx -\frac{\mu}{1-\mu}\frac{1}{1-x} + \frac{4\lambda}{(1-\mu)^2}\frac{x}{(1-x)^2}, \tag{2.16}$$

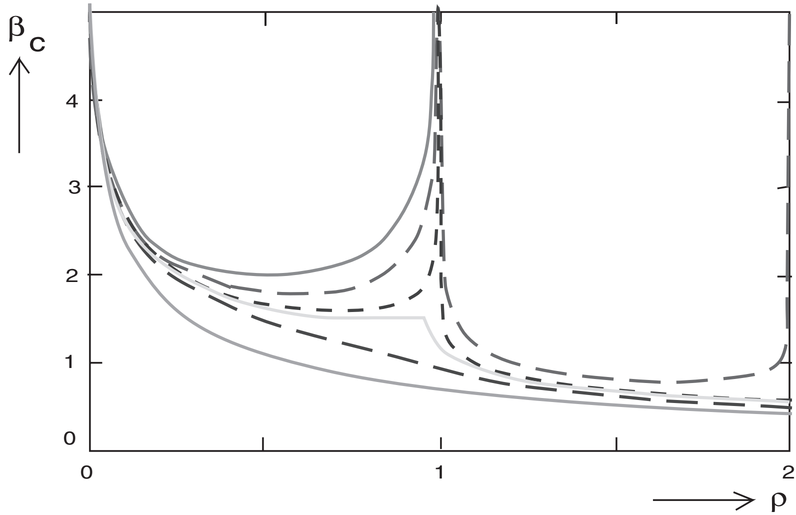

Fig. 3. The critical inverse temperature for a number of values of the coupling strength λ. The lower curve is for the free lattice gas: $\lambda = 0$, the top curve is for the case of complete single-site exclusion $\lambda = +\infty$. Intermediate values are, from the bottom up: $\lambda = 2$, 2.5, 3, and 5.

where $x = e^{\beta(\mu-1)}$. Therefore, at $\beta = \beta_c$,

$$\frac{x}{1-x} = \frac{\mu(1-\mu)}{4\lambda}. \tag{2.17}$$

On the other hand, the same approximation in (2.15) yields

$$\rho \approx \frac{x}{1-x}. \tag{2.18}$$

Combining the two equations we see that we must have $\mu < 1$ and $16\rho\lambda < 1$. Solving for μ we have $\mu = \frac{1}{2}(1 - \sqrt{1-16\rho\lambda})$ and

$$\beta_c \approx \frac{2}{1+\sqrt{1-16\lambda\rho}} \ln\left(\frac{1}{\rho}+1\right). \tag{2.19}$$

In the limit $\lambda \to 0$ this clearly agrees with the free Bose gas limit $\beta_c^{\text{free}}(\rho) = \ln(1+\frac{1}{\rho})$.

On the other hand, for large μ, a careful asymptotic analysis of (2.10) shows that the asymptotic behavior of β_c is given by

$$\beta_c \approx \frac{2\lambda}{\mu} \qquad (\mu \gg 1 > \lambda). \tag{2.20}$$

For large μ, i.e., for large densities ρ, Eq. (2.15) implies that

$$\rho = \rho(\beta, \mu) \approx \frac{\mu + \lambda - 1}{2\lambda} \qquad (\rho \gg 1),$$

(see the straight line of Fig. 2). Combined with (2.20) we get

$$\beta_c \approx 1/\rho \qquad (\rho \gg 1), \tag{2.21}$$

which corresponds also to the free Bose gas limit $\beta_c^{\text{free}}(\rho)$ at large densities ρ.

We proceed to compute the pressure p as a function of the density. For this, we need 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

$$\langle n|\, e^{r(a+a^*)}\, |m\rangle = \sqrt{n!m!} \sum_{k=0}^{n \wedge m} \frac{r^{n+m-2k}}{k!\,(n-k)!\,(m-k)!}\, e^{r^2/2}. \tag{2.22}$$

The resulting graphs, for several values of λ and for $\beta = 2$ are depicted in Figs. 4 and 5.

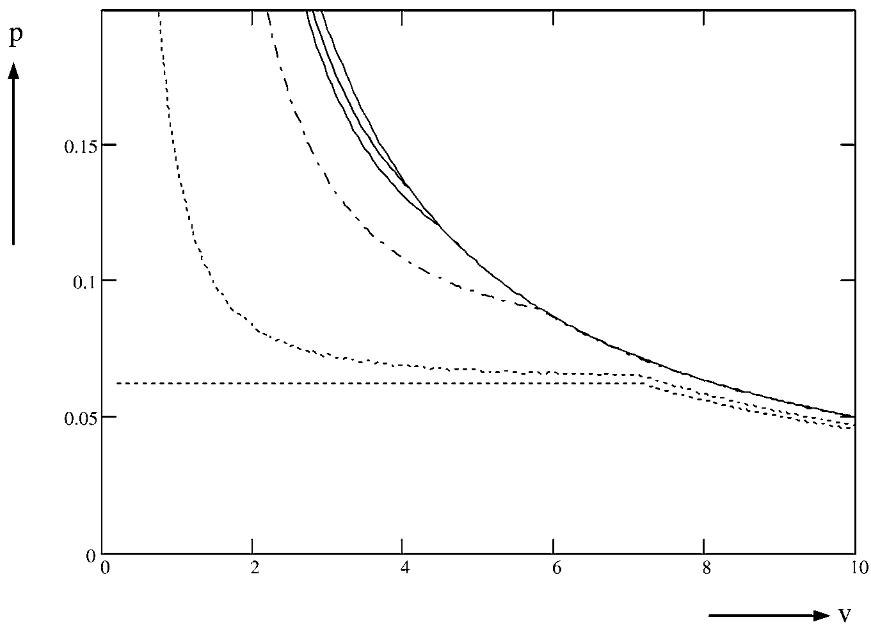

Fig. 4. The pressure vs. specific volume diagram for $\beta = 2.1$ and $\lambda = 0$ (free gas, lower graph), 0.1, 1, 3, 5, and $+\infty$.

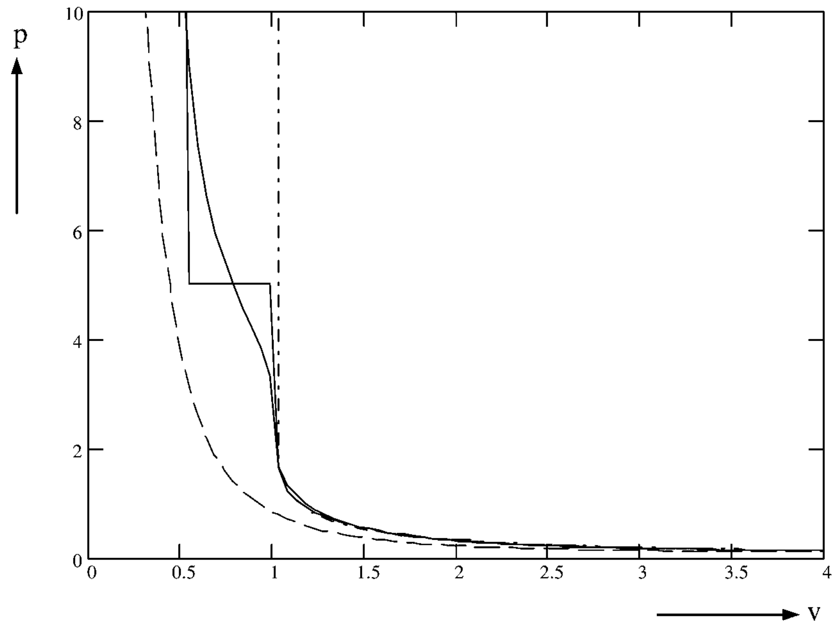

Fig. 5. The pressure vs. specific volume diagram at higher values of the pressure. The dashed line is the free gas. The graph with s-bend corresponds to $\lambda = 3$, the graph with horizontal section corresponds to $\lambda = 5$, the dashed dotted line is $\lambda = +\infty$.

Figure 4 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 Fig. 3 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 Fig. 5, but occurs at much higher pressures and cannot, therefore, be seen at the scale of Fig. 4.

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: see Fig. 6.

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 Fig. 7. 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. This is, so far, unexplained.

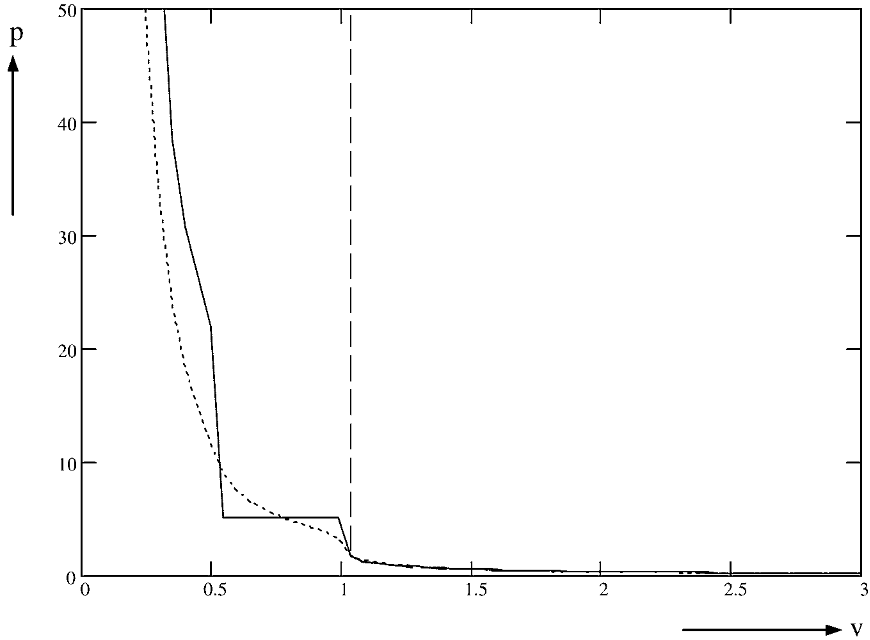

Fig. 6. The pressure vs. specific volume diagram at still higher values of the pressure. The dotted line corresponds to $\lambda = 3$ whereas the solid one is for $\lambda = 5$.

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 Fig. 8.

As previously announced, the suppression of Bose–Einstein condensation for $\lambda_k < \lambda < \lambda_{k+1}$ at densities near the integer values $\rho = 1, \ldots, k$ corresponds to a "Mott insulator phase," where we find an energy gap to all excitations (cf. (2.13) and (2.14)). This phase transition was found previously in refs. 3–8, but only at zero-temperature, where it is called a quantum phase transition. Here we have obtained the phase diagram for arbitrary temperature.

An intuitive explanation for the suppression of Bose–Einstein condensation near 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 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 for the existence of a "Mott insulator

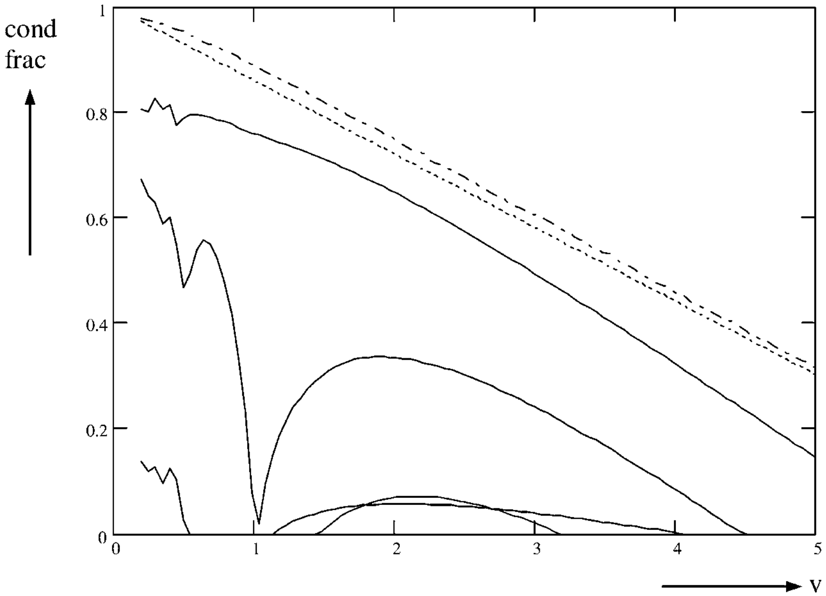

Fig. 7. The condensate fraction as a function of the specific volume for several interaction strengths. The dotted straight line is the free gas ($\lambda = 0$) condensate fraction. The dashed dotted line just above this corresponds to $\lambda = 0.1$. Subsequent graphs correspond to $\lambda = 1, 3, 5$ and $+\infty$ from top to bottom. The condensate fraction for $\lambda = 5$ occurs for $v < 0.5$ and $1.2 < v < 4$. Notice also the oscillation of the condensate fraction due to partial suppression of the condensate at intermediate values of the density for $\lambda = 1, 3, 5$.

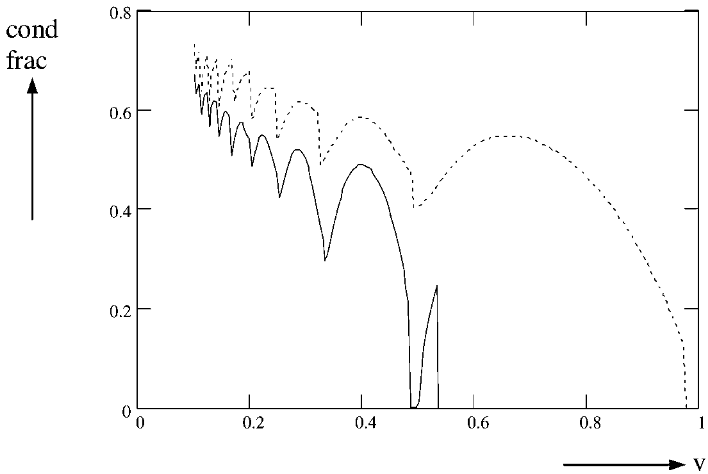

Fig. 8. The condensate fraction for $\lambda = 3$ (dashed line) and $\lambda = 5$ (solid line).

phase" 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. (In the presence of an external potential given by $\sum_x \epsilon_x n_x$ (cf. (1.1)) this argument is no longer strictly applicable, but in the region where ϵ_x is nearly constant, the variation of the potential would be less than the energy gap and one may nevertheless expect the phenomenon to persist.)

In their experiment, Greiner *et al.*[1] were able to experimentally change the parameter $\lambda = U/2J$ by modifying the optical lattice potential depth. They were thus able to go from the Bose condensation phase to the Mott insulator phase and back, i.e., to cross the critical value $\lambda_{c,1}$, concluding that the phenomenon is reversible.

Our detailed analysis shows that, for strong repulsion, there are several singularities in the pressure-volume lines (Figs. 4, 5, and 6) at different pressure scales. It would be interesting if these features could be observed experimentally. However, the dilute-gas experiments of ref. 1 and others are not suitable for this purpose as it is impossible to reach sufficiently high pressures and densities. Solid-state systems may be more promising in this regard.

APPENDIX A

Let

$$c_0 \equiv \frac{1}{\sqrt{V}} \sum_{x=1}^{V} a_x, \tag{A.1}$$

$$H_V^0 \equiv \sum_{x=1}^{V} n_x + \lambda \sum_{x=1}^{V} n_x(n_x - 1), \tag{A.2}$$

$$N_V \equiv \sum_{x=1}^{V} n_x, \tag{A.3}$$

$$p_V(\beta, \mu) \equiv \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathscr{F}_B} \{e^{-\beta(H_V - \mu N_V)}\}, \tag{A.4}$$

where $\mathscr{F}_B$ is the corresponding boson Fock space. Note that (1.2) can be written as

$$H_V = -c_0^* c_0 + H_V^0. \tag{A.5}$$

Define the "approximating Hamiltonian" as a function of the complex parameter z by:

$$H_V^I(z) \equiv V\,|z|^2 - z\sqrt{V}\, c_0^* - \bar{z}\sqrt{V}\, c_0 + H_V^0. \tag{A.6}$$

Then,

$$H_V^I(z) - H_V = V\left(\frac{c_0^*}{\sqrt{V}} - \bar{z}\right)\left(\frac{c_0}{\sqrt{V}} - z\right) \geqslant 0. \tag{A.7}$$

Let

$$p_V^I(\beta, \mu, z) \equiv \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathscr{F}_B}\{e^{-\beta(H_V^I(z) - \mu N_V)}\}. \tag{A.8}$$

To find the thermodynamic limit of $p_V(\beta, \mu)$ (A.4) we follow the idea of paper[19] where the author proves the exactness of the Bogoliubov approximation for a non-ideal Bose-gas with superstable interaction.[29]

First, we introduce the Hamiltonians $H_V(v)$ and $H_V^I(v, z)$ respectively by

$$\begin{aligned} H_V(v) &= H_V - \sqrt{V}\,(\bar{v}c_0 + v c_0^*), \\ H_V^I(v, z) &= H_V^I(z) - V(\bar{v}z + v\bar{z}). \end{aligned} \tag{A.9}$$

with source $v \in \mathbb{C}$. Let $p_V(\beta, \mu, v)$ and $p_V^I(\beta, \mu, v, z)$ the two corresponding pressures. By the Bogoliubov inequality[18, 29] for $H_V(v)$ and $H_V^I(v, z)$, one has:

$$\begin{aligned} 0 &\leqslant \inf_{z \in \mathbb{C}} \{p_V(\beta, \mu, v) - p_V^I(\beta, \mu, v, z)\} \\ &\leqslant \frac{1}{V} \langle (c_0^* - \sqrt{V}\,\bar{z}_0)(c_0 - \sqrt{V}\,z_0)\rangle_{H_V(v)}, \end{aligned} \tag{A.10}$$

for any complex parameter z_0, see (A.7). Defining

$$\delta_0 = c_0 - \langle c_0 \rangle_{H_V(v)}$$

we have $[\delta_0, \delta_0^*] = 1$ and hence

$$\delta_0^* \delta_0 = \tfrac{1}{2}\{\delta_0^*, \delta_0\} - 1,$$

with $\{X, Y\} \equiv XY + YX$. The inequality (A.10) then implies:

$$0 \leqslant p_V(\beta, \mu, v) - \sup_{z \in \mathbb{C}} p_V^I(\beta, \mu, v, z) \leqslant \frac{1}{2V} \langle \{\delta_0^*, \delta_0\} \rangle_{H_V(v)}. \tag{A.11}$$

for $z_0 = \langle c_0 \rangle_{H_V(v)} / \sqrt{V}$. From a spectral decomposition of the Hamiltonian $H_V(\mu, v) \equiv H_V(v) - \mu N_V$:

$$H_V(\mu, v)\, \psi_n = E_n \psi_n,$$

one obtains

$$\langle\{\delta_0^*, \delta_0\}\rangle_{H_V(\nu)} = e^{-\beta V p_V(\beta, \mu, \nu)} \sum_{m, n} |A_{mn}|^2 \left(e^{-\beta E_n} + e^{-\beta E_m}\right), \tag{A.12}$$

with $A_{mn} = (\psi_m, \delta_0 \psi_n)$. Notice that

$$\begin{aligned}
(e^{-\beta E_n} + e^{-\beta E_m}) &= 2 \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\beta(E_m - E_n)} \frac{\beta(E_m - E_n)}{2} \frac{(e^{-\beta E_n} + e^{-\beta E_m})}{(e^{-\beta E_n} - e^{-\beta E_m})} \\
&= 2 \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\beta(E_m - E_n)} \frac{\beta(E_m - E_n)}{2} \coth\left(\frac{\beta(E_m - E_n)}{2}\right).
\end{aligned}$$

The inequality

$$\cosh x - \frac{\sinh x}{x} = \sum_{n=1}^{\infty} \frac{2n}{(2n+1)!} x^{2n} \leqslant \frac{x \sinh x}{3},$$

implies that $x \coth x \leqslant 1 + x^2/3$ for all real x. So, we obtain for (A.12) the following upper bound:

$$\begin{aligned}
\langle\{\delta_0^*, \delta_0\}\rangle_{H_V(\nu)} \leqslant{}& 2e^{-\beta V p_V(\beta, \mu, \nu)} \sum_{m, n} |A_{mn}|^2 \frac{(e^{-\beta E_n} - e^{-\beta E_m})}{\beta(E_m - E_n)} \\
&+ \frac{1}{6} e^{-\beta V p_V(\beta, \mu, \nu)} \sum_{m, n} |A_{mn}|^2 (e^{-\beta E_n} - e^{-\beta E_m})\, \beta(E_m - E_n).
\end{aligned} \tag{A.13}$$

In terms of the Bogoliubov scalar product $(.,.)_H$ defined by (2.4) for $H = H_V(\nu)$, the inequality (A.13) can be written as

$$\frac{1}{2} \langle\{\delta_0^*, \delta_0\}\rangle_{H_V(\nu)} \leqslant (\delta_0, \delta_0)_{H_V(\nu)} + \frac{\beta}{12} \langle[\delta_0^*, [H_V(\mu, \nu), \delta_0]]\rangle_{H_V(\nu)}. \tag{A.14}$$

(This inequality had already been proven in ref. 30, see also ref. 17). From

$$\sum_{x=1}^{V} [c_0^*, [n_x^2, c_0]] = \frac{1}{V} \sum_{x=1}^{V} (4n_x + 1),$$

$$\sum_{x=1}^{V} [c_0^*, [n_x, c_0]] = 1, \qquad [c_0^*, [c_0^* c_0, c_0]] = 1,$$

one has

$$[\delta_0^*, [H_V(\mu, \nu), \delta_0]] = [c_0^*, [H_V(\mu, \nu), c_0]] = -[c_0^*, [c_0^* c_0, c_0]] + (1-\mu-\lambda) \sum_{x=1}^{V} [c_0^*, [n_x, c_0]] + \lambda \sum_{x=1}^{V} [c_0^*, [n_x^2, c_0]] = -\mu + \frac{4\lambda N_V}{V}.$$

We now use the fact that the model H_V is superstable. In fact by the Cauchy–Schwarz inequality,

$$H_V - \mu N_V \geqslant -(\lambda+\mu)\, N_V + \lambda \frac{N_V^2}{2V}.$$

It follows that the pressure $p_V(\beta, \mu, \nu)$ is defined for any $\mu \in \mathbb{R}$ and $\nu \in \mathbb{C}$ and the solution $\hat{z}_V(\beta, \mu, \nu)$ of

$$\sup_{z \in \mathbb{C}} p_V^I(\beta, \mu, \nu, z) = p_V^I(\beta, \mu, \nu, \hat{z}_V(\beta, \mu, \nu))$$

satisfies $|\hat{z}_V(\beta, \mu, \nu)|^2 \leqslant (\lambda+\mu_0)/\lambda$ for $\mu \leqslant \mu_0$ and $|\nu| \leqslant r_0$. Note also that

$$\left\langle \frac{c_0}{\sqrt{V}} \right\rangle_{H_V(\nu)} \left\langle \frac{c_0^*}{\sqrt{V}} \right\rangle_{H_V(\nu)} \leqslant \left\langle \frac{c_0^* c_0}{V} \right\rangle_{H_\Lambda(\nu)} \leqslant \left\langle \frac{N_V}{V} \right\rangle_{H_V(\nu)} = \partial_\mu p_V(\beta, \mu, \nu).$$

Now, since $p_V(\beta, \mu, \nu)$ is a convex function of μ and also of $|\nu|$, there is a uniform bound

$$M = \max\{\partial_\mu p_V(\beta, \mu_0, r_0), B/C\}$$

such that

$$\begin{cases} (\langle c_0/\sqrt{V} \rangle_{H_V(\nu)} (\beta, \mu))^2 \leqslant \langle N_V/V \rangle_{H_V(\nu)} (\beta, \mu) \leqslant M, \\ |\hat{z}_V(\beta, \mu, \nu)|^2 \leqslant M, \end{cases} \tag{A.15}$$

for $\mu \leqslant \mu_0$ and $|\nu| \leqslant r_0$. Therefore, there exist u and w such that the estimate (A.11) for $\mu \leqslant \mu_0$ becomes:

$$0 \leqslant p_V(\beta, \mu, \nu) - \sup_{z \in \mathbb{C}} p_V^I(\beta, \mu, \nu, z) \leqslant \frac{1}{V} [u + w(\delta_0^*, \delta_0)_{H_V(\nu)}]. \tag{A.16}$$

Now we can reason along the standard lines of the Approximation Hamiltonian Method (see refs. 17 and 18). First we note that

$$(\delta_0, \delta_0)_{H_V(v)} = \frac{1}{\beta}\, \partial_v \partial_{\bar{v}}\, p_V[H_V(v)]. \tag{A.17}$$

By the (canonical) gauge transformation $c_0 \to c_0 e^{i\varphi}$, $\varphi = \arg v$, one finds that in fact

$$p_V[H_V(v)] = p_V(\beta, \mu; |v| \equiv r).$$

Then passing in (A.17) to polar coordinates (r, φ) we obtain:

$$(\delta_0, \delta_0)_{H_V(v)} = \frac{1}{4\beta r}\, \partial_r (r \partial_r\, p_V). \tag{A.18}$$

Let $z = |z|\, e^{i\psi}$, $\psi = \arg z$. Then from (A.9), we obtain

$$\begin{aligned} p_V(\beta, \mu, v) - \sup_{z \in \mathbb{C}}\, p_V^I(\beta, \mu, v, z) &= p_V(\beta, \mu, v) - \sup_{|z|, \psi}\, p_V^I(\beta, \mu, r e^{\pm i\varphi}, |z|\, e^{\pm i\psi}) \\ &= p_V(\beta, \mu, v) - \sup_{|z|}\, p_V^I(\beta, \mu, r, |z|\, e^{\pm i\varphi}) \\ &\equiv \inf_{|z|}\, \Delta_V(r). \end{aligned} \tag{A.19}$$

Consequently, by (A.16) we find that

$$\int_R^{R+\varepsilon} r \inf_{|z|}\, \Delta_V(r)\, dr \leqslant \frac{1}{V} \left\{ u\, \frac{(2R+\varepsilon)\, \varepsilon}{2} + \frac{w}{4\beta}\, (r \partial_r\, p_V) \Big|_R^{R+\varepsilon} \right\}, \tag{A.20}$$

for $[R, R+\varepsilon] \subset [0, r_0]$. Note that by (A.15) we have

$$\partial_r\, p_V = 2\, |\langle c_0 / \sqrt{V} \rangle_{H_V(v)}| \leqslant 2 \sqrt{M}, \qquad \mu \in C_0 \subset \mathbb{R},\ |v| \leqslant r_0. \tag{A.21}$$

Therefore (A.20) takes the form

$$\int_R^{R+\varepsilon} r \inf_{|z|}\, \Delta_V(r)\, dr \leqslant \frac{1}{V} \left\{ u\, \frac{(R+\varepsilon)^2 - R^2}{2} + \frac{w}{2\beta} \sqrt{M}\, (2R+\varepsilon) \right\}. \tag{A.22}$$

By (A.15), we obtain

$$|\partial_r \inf_{|z|}\, \Delta_V(r)| \leqslant 4 \sqrt{M}, \qquad (r \in [R, R+\varepsilon]),$$

which implies

$$\inf_{|z|} \Delta_V(R) \leqslant \inf_{|z|} \Delta_V(r) + 4\sqrt{M}\,(r-R).$$

Hence,

$$\inf_{|z|} \Delta_V(R)\,\frac{(R+\varepsilon)^2 - R^2}{2} \leqslant \int_R^{R+\varepsilon} r \inf_{|z|} \Delta_V(r)\,dr + 4\sqrt{M}\left(\frac{r^3}{3} - R\frac{r^2}{2}\right)\Big|_R^{R+\varepsilon},$$

and by (A.22), we find

$$\inf_{|z|} \Delta_V(R) \leqslant \frac{1}{V}\left\{u + \frac{w}{\beta}\sqrt{M}\,\varepsilon^{-1}\right\} + 2\sqrt{M}\,\varepsilon\,\frac{R+\frac{2}{3}\varepsilon}{R+\frac{1}{2}\varepsilon}. \tag{A.23}$$

Since $\varepsilon > 0$ is still arbitrary, in the thermodynamic limit one gets the optimal value for the right-hand side of (A.23) by taking $\varepsilon \sim 1/\sqrt{V}$. Then, for large V we obtain from (A.23) the following estimate:

$$0 \leqslant p_V(\beta, \mu, \nu) - \sup_{z \in \mathbb{C}} p_V^I(\beta, \mu, \nu, z) \leqslant \frac{\text{const}}{\sqrt{V}}, \tag{A.24}$$

which is valid for $\mu < \mu_0$ and $|\nu| \leqslant r_0$. Since μ_0 is also arbitrary, for $\nu = 0$, we deduce

$$p(\beta, \mu) = \sup_{z \in \mathbb{C}} p^I(\beta, \mu, z), \tag{A.25}$$

for any fixed $\mu \in \mathbb{R}$. Now notice that $H_V^I(z)$ is in fact a sum over x of independent terms and the trace in (A8) decouples. The result is

$$p^I(\beta, \mu, z) = -|z|^2 + \frac{1}{\beta} \ln \operatorname{Trace} \exp\left[\beta((\mu-1)\,n - \lambda n(n-1) + (za^* + \bar{z}a))\right], \tag{A.26}$$

where we recall that the trace is over the representation space of a single oscillator with creation and annihilation operators a^* and a, and $n = a^*a$. Finally, using the gauge transformation

$$\mathcal{U}_\varphi\, a\mathcal{U}_\varphi^* = ae^{-i\varphi} = \tilde{a}, \qquad \varphi = \arg z,$$

combined with (A.25) and (A.26) we get (1.4).

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