C^*-ALGEBRAIC APPROACH TO THE BOSE-HUBBARD MODEL

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Abstract: We give a new derivation of the variational formula for the pressure of the long-range-hopping Bose-Hubbard model, which was first proved in [1]. The proof is analogous to that of a theorem on noncommutative large deviations introduced by Petz, Raggio and Verbeure [2] and could similarly be extended to more general Bose system of mean-field type. We apply this formalism to prove Bose-Einstein condensation for the case of small coupling.

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1. Introduction

The Bose-Hubbard Model with nearest-neighbour hopping is defined on a cubic lattice $\mathbb{Z}^d$ of dimension d by the Hamiltonian

$$H = \frac{1}{2} \sum_{x,y\in\mathbb{Z}^d :\, |x-y|=1} (a_x^* - a_y^*)(a_x - a_y) + \lambda \sum_x n_x(n_x - 1), \tag{1.1}$$

where the operators a_x^* and a_x are creation and annihilation operators satisfying the usual bosonic commutation relations

$$[a_x, a_y^*] = \delta_{x,y}.$$

The operators $n_x = a_x^* a_x$ are the local number operators.

In [1] a long-range-hopping version of this model was analysed. It is given by the Hamiltonian

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

on a complete graph of V sites. In particular, the following variational expression for the pressure was derived:

$$p(\beta,\mu,\lambda) = \sup_{r\geq 0} \Big\{ -r^2 + \frac{1}{\beta} \ln \mathrm{Tr} \exp \Big[\beta \Big((\mu + \lambda - 1)n - \lambda n^2 + r(a + a^*) \Big) \Big] \Big\}. \tag{1.3}$$

The derivation made use of the so-called approximating Hamiltonian method introduced by Bogoliubov Jr. [3] and made rigorous by Zagrebnov et al. [4], see also [5]. Here we present a new derivation of this formula using the C*-algebraic method of Petz, Raggio and Verbeure [2], which is inspired in part by Varadhan's theorem in probabilistic large deviation theory, and in part by work of Fannes, Spohn and Verbeure [6]. Our C*-algebraic approach corresponds to variational expressions for thermodynamic functionals of classical Gibbs measures [7], and in particular we are using the variational expression for the relative entropy (see [8] for classical probability theory). As a result we obtain a variational expression for the pressure where we optimize over states of the infinite system. Due to the symmetry (lack of geometry) on the complete graph this expression can be simplified to (1.3) using the well-known Størmer theorem. Hence, our results here are a quantum analogy of recent results for classical statistical mechanical models on complete graphs using exchangeability [9]. The analysis in [2] concerns quantum spin models and the extension to the Bose-Hubbard model requires a number of technical considerations. Many of these can be found in the book by Ohya and Petz [10], but we present some of the proofs here nonetheless in order to make this paper more self-contained.

Section 2 contains the proof of our variational formula (1.3). In Section 3 we briefly present some of the features of the model again, mainly in order to correct some minor but irritating errors in the analysis of [1]. In Section 4, we show that some of the C*-algebraic formalism extends to the nearest-neighbour hopping model, resulting in a variational formula for the pressure analogous to the well-known formula for spin models. This formula does not appear to have been written down before. As the variation is over the set of all translation-invariant states on the lattice, it is difficult to analyse, however, just as in the case of spin models.

2. C*-algebraic derivation

We follow the technique of Petz, Raggio and Verbeure [2]. The Hamiltonian is invariant under the permutation group. We write it as

$$H_V = -V\Big(\frac{1}{V}\sum_{x=1}^{V} a_x^*\Big)\Big(\frac{1}{V}\sum_{y=1}^{V} a_y\Big) + \sum_{x=1}^{V} h_x, \tag{2.1}$$

where

$$h_x = n_x + \lambda n_x(n_x - 1).$$

For finite V we thus assume that a CCR algebra $\mathcal{A}_V$ is given generated by creation and annihilation operators a_x^* and a_x ($x \in \{1, \dots, V\}$) and with standard representation on the Fock space $\mathcal{F}_V$.

Next we define a reference state ω_V on the Fock space $\mathcal{F}_V$ as the product state $\omega_V = \bigotimes_{x=1}^{V} \omega_x$, where ω_x has the density matrix

$$\rho_{\omega_x} = \frac{\exp[\beta(\mu n_x - h_x)]}{\operatorname{Tr}\exp[\beta(\mu n_x - h_x)]}.$$

Let

$$\mathcal{A} = \overline{\bigcup_{V=1}^{\infty} \mathcal{A}_V} \tag{2.2}$$

be the (quasi-local) CCR algebra for the complete lattice $\mathbb{N}$, where the closure is taken with respect to the norm topology.

Lemma 2.1. *Suppose that ϕ is a regular permutation-invariant state on $\mathcal{A}$ such that $\phi(n_x) < +\infty$ for all $x \in \{1, \dots, V\}$. Then*

$$\lim_{V\to\infty} \phi\Big(\Big(\frac{1}{V}\sum_{x=1}^{V} a_x^*\Big)\Big(\frac{1}{V}\sum_{y=1}^{V} a_y\Big)\Big) = \phi(a_1^* a_2).$$

Proof. Notice that we can define $\phi(n_x)$ as the supremum

$$\phi(n_x) = \sup_{N\geq 1} \phi(P_N^{(x)} n_x),$$

where $P_N^{(x)}$ is the projection on the subspace of $\mathcal{F}_x$ with $n_x \leq N$. Obviously, this is independent of x by permutation invariance. The formula $\phi\big(\big(\frac{1}{V}\sum_{x=1}^V a_x^*\big)\big(\frac{1}{V}\sum_{y=1}^V a_y\big)\big)$ should be interpreted in a similar way:

$$\phi\Big(\Big(\frac{1}{V}\sum_{x=1}^V a_x^*\Big)\Big(\frac{1}{V}\sum_{y=1}^V a_y\Big)\Big) = \sup_{N\geq 1}\phi\Big(\frac{1}{V^2}P_N^V\sum_{x,y=1}^V a_x^* a_y P_N^V\Big),$$

where

$$P_N^V = \bigotimes_{x\in V} P_N^{(x)}.$$

We now write

$$\begin{aligned}
&\phi\Big(\Big(\frac{1}{V}\sum_{x=1}^V a_x^*\Big)\Big(\frac{1}{V}\sum_{y=1}^V a_y\Big)\Big) = \\
&= \sup_{N\geq 1}\frac{1}{V^2}\Big\{\sum_{x=1}^V \phi\big(P_N^V n_x\big) + \sum_{x\neq y}\phi\big(P_N^V a_x^* a_y P_N^V\big)\Big\}.
\end{aligned}$$

The first term is clearly bounded by $\frac{1}{V}\phi(n_x)$ and hence tends to zero. By permutation invariance, the second term equals

$$\frac{V-1}{V}\phi\left(P_N^V a_1^* a_2 P_N^V\right).$$

We conclude by proving that the limit (first $N\to\infty$ and subsequently $V\to\infty$) of this expression exists and equals

$$\phi(a_1^*a_2) = \lim_{N\to\infty}\phi(P_N^{(1)}a_1^*P_N^{(1)}P_N^{(2)}a_2P_N^{(2)}). \tag{2.3}$$

To this end we write

$$\begin{aligned}
&\phi(P_{N_1}^V a_1^* a_2 P_{N_1}^V) - \phi(P_{N_2}^V a_1^* a_2 P_{N_2}^V) \\
&\quad = \phi\left((P_{N_1}^V - P_{N_2}^V)a_1^*a_2P_{N_1}^V\right) + \phi\left(P_{N_2}^V a_1^* a_2 (P_{N_1}^V - P_{N_2}^V)\right)
\end{aligned}$$

and treat each term separately. Both terms are similar; we consider only the first. We have

$$\begin{aligned}
&|\phi\left((P_{N_1}^V - P_{N_2}^V)a_1^*a_2P_{N_1}^V\right)| \\
&\quad\leq \left[\phi\left((P_{N_1}^V - P_{N_2}^V)a_1^*a_1(P_{N_1}^V - P_{N_2}^V)\right)\right]^{1/2}\left[\phi\left(P_{N_1}^V a_2^* a_2 P_{N_1}^V\right)\right]^{1/2}.
\end{aligned}$$

The second factor is obviously bounded by $\phi(n_2)^{1/2}$. In the first factor we can write

$$\begin{aligned}
P_{N_1}^V - P_{N_2}^V &= (P_{N_1}^{(1)} - P_{N_2}^{(1)})\otimes P_{N_1}^{(2)}\otimes\cdots\otimes P_{N_1}^{(V)} \\
&\quad + \cdots + P_{N_2}^{(1)}\otimes\cdots\otimes P_{N_2}^{(V-1)}\otimes(P_{N_1}^{(V)} - P_{N_2}^{(V)}).
\end{aligned}$$

With the observation that $P^V_{N_1} - P^V_{N_2}$ commutes with $a_1^* a_1$ we get

$$\begin{aligned}&\phi((P^V_{N_1} - P^V_{N_2})a_1^* a_1(P^V_{N_1} - P^V_{N_2}))\\ \leq\ &\phi((P^{(1)}_{N_1} - P^{(1)}_{N_2})a_1^* a_1(P^{(1)}_{N_1} - P^{(1)}_{N_2})) + (V-1)\phi(P^{(x)}_{N_1} - P^{(x)}_{N_2}),\end{aligned}$$

and therefore the limit of $P^V_N a_x^* a_y P^V_N$ exists. Similarly, one proves that

$$\left|\phi(P^V_{N_1} a_1^* a_2 P^V_{N_1}) - \phi(P^{(1)}_N a_1^* P^{(1)}_N P^{(2)}_N a_2 P^{(2)}_N)\right| \to 0$$

for fixed V. Taking the limit $N \to \infty$ and subsequently $V \to \infty$ the result follows. □

Remark 2.2. Since ϕ is regular, its restriction ϕ_V to each $\mathcal{A}_V$ is regular, and the number operators n_x are well-defined. Moreover, the corresponding GNS representation is equivalent with the Fock representation by Von Neumann's theorem [11]. In particular, ϕ_V is normal for all V, i.e. ϕ is locally normal. Thus ϕ_V has a density matrix ρ_{ϕ_V}.

Lemma 2.1 gives the mean energy for our model. Next we are concerned with the relative entropy with respect to our reference state ω_V. It is well-known that the relative entropy

$$S(\phi_V \,\|\, \omega_V) = \mathrm{Tr}\,[\rho_{\phi_V}(\ln \rho_{\phi_V} - \ln \rho_{\omega_V})]$$

is convex and superadditive [10]. A precise definition of $S(\phi \,\|\, \omega)$ for states on a Von Neumann algebra was given by Araki [12, 13]. Given the standard representation π of $\mathcal{B}(\mathcal{F}_V)$ (the GNS representation with respect to the tracial state) one has

$$S(\phi_V \,\|\, \omega_V) = -\langle \Phi_V|\, \ln \Delta_{\Omega_V,\Phi_V}\, |\Phi_V\rangle, \tag{2.4}$$

where

$$\Delta_{\Omega_V,\Phi_V} = \pi(\rho_{\omega_V})\pi'(\rho_{\phi_V})^{-1}$$

is the *relative modular operator*. Here $\Phi_V = \rho^{1/2}_{\phi_V}$ and $\Omega_V = \rho^{1/2}_{\omega_V}$ respectively, and hence $\phi_V(A) = \langle \Phi_V|\pi(A)\Phi_V\rangle$ and $\omega_V(A) = \langle \Omega_V, \pi(A)\Omega_V\rangle$. If $E_{\Omega,\Phi}$ is the corresponding resolution of the identity, then we can write

$$\begin{aligned}S(\phi_V \,\|\, \omega_V) &= -\int_0^1 \ln\lambda\, \langle \Phi_V|\, E_{\Omega_V,\Phi_V}(\mathrm{d}\lambda)\, |\Phi_V\rangle\\ &\quad - \int_1^\infty \ln\lambda\, \langle \Phi_V|\, E_{\Omega_V,\Phi_V}(\mathrm{d}\lambda)\, |\Phi_V\rangle.\end{aligned} \tag{2.5}$$

Here we have separated the two integration domains to indicate that the second integral is always convergent, whereas the first should be interpreted as

$$-\inf_{\delta>0} \int_\delta^1 \ln\lambda\, \langle \Phi_V|\, E_{\Omega_V,\Phi_V}(\mathrm{d}\lambda)\, |\Phi_V\rangle$$

and determines whether $S(\phi_V \,\|\, \omega_V)$ is finite or infinite. Note that $S(\phi_V \,\|\, \omega_V) = +\infty$ if $\Phi_V \not\leq \mathrm{supp}\,(\omega_V)$.

An equivalent definition was introduced by Uhlmann [14]:

$$S(\phi_V \,\|\, \omega_V) = -\lim_{t\downarrow 0} \frac{1}{t}\left(\|\Delta^{t/2}_{\Omega_V,\Phi_V}\Phi_V\|^2 - 1\right). \tag{2.6}$$

This is easily seen to be equivalent using Lebesgue's monotone convergence theorem. We now prove the following variational formula for the relative entropy (compare [8, Lemma 3.2.13] for classical probability theory):

Theorem 2.3. *For any state ϕ_V on $\mathcal{B}(\mathcal{F}_V)$,*

$$\begin{aligned} S(\phi_V \,\|\, \omega_V) = & \sup_{A\in\mathcal{B}(\mathcal{F}_V)\colon A^*=A} \left\{\beta\phi_V(A) - \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + A)}\right\} \\ & + V \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n_1 - h_1)}. \end{aligned}$$

Proof. We first prove that $S(\phi_V \,\|\, \omega_V)$ is greater than the right-hand side. Let $A \in \mathcal{B}(\mathcal{F}_V)$ be self-adjoint. Then we can define the perturbed state ψ_V by

$$\rho_{\psi_V} = \frac{\mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + A)}}{\operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + A)}}.$$

We write

$$Z_{A,V} = \operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + A)}$$

and $Z_V = \operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x}$ in the following. We employ a change of state (measure) method [8] with respect to the reference state ω_V and the perturbed reference state ψ_V. The non-commutativity of our random variables is an additional difficulty. But the Du Hamel formula gives

$$\begin{aligned} &\langle \Phi_V |\, \Delta^t_{\Psi_V,\Phi_V} \,|\Phi_V\rangle \\ &= Z_{A,V}^{-t} Z_V^t \Big\langle \Phi_V |\, \Big(1\!\!1 - \beta \int_0^t \mathrm{d}\tau \, \pi(\mathrm{e}^{-\beta\tau H_V^A} A \mathrm{e}^{\beta\tau H_V^0}\Big) \pi(\rho^t_{\omega_V}) \pi'(\phi_V^{-t}) |\Phi_V\Big\rangle. \end{aligned} \tag{2.7}$$

where

$$H_V^A = -\mu\mathcal{N} + \sum_{x=1}^V h_x - A,$$

and where $H_V^0 = -\mu\mathcal{N} + \sum_{x=1}^V h_x$ is the non-interacting part of the Hamiltonian in (2.1). Differentiating we get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0^+} \langle \Phi_V |\, \Delta^t_{\Psi_V,\Phi_V} \,|\Phi_V\rangle = & -\ln Z_{A,V} + \ln Z_V - \beta\langle \Phi_V |\, \pi(A)\Phi_V\rangle \\ & + \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0^+} \langle \Phi_V |\, \Delta^t_{\Omega_V,\Phi_V} \,|\Phi_V\rangle \end{aligned} \tag{2.8}$$

and hence

$$S(\phi_V \,\|\, \psi_V) = S(\phi_V \,||\, \omega_V) - \beta\phi_V(A) + \ln \frac{\operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + A)}}{\operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x)}}. \tag{2.9}$$

The desired inequality now follows from the positivity of the relative entropy. (Notice that this follows immediately from $\ln\lambda \leq 1-\lambda$ and

$$\int \lambda\langle\Phi_V|\, E_{\Psi_V,\Phi_V}(\mathrm{d}\lambda)\,|\Phi_V\rangle = \langle\Phi_V|\,\Delta_{\Psi_V,\Phi_V}\,|\Phi_V\rangle$$
$$= \langle\Phi_V|\,\pi(\rho_{\psi_V})\pi'(\rho_{\phi_V})^{-1}\,|\Phi_V\rangle = \mathrm{Tr}(\rho_{\psi_V}) = 1$$

by a simple approximation.)

To prove the converse inequality, first assume that $c_1\omega_V \leq \phi_V \leq c_2\omega_V$ for constants $0 < c_1 < c_2 < +\infty$. Then there exists a bounded relative Hamiltonian A such that

$$\rho_{\phi_V} = \frac{\mathrm{e}^{\beta(\mu\mathcal{N}-\sum_{x=1}^{V} h_x + A)}}{\mathrm{Tr}\,\mathrm{e}^{\beta(\mu\mathcal{N}-\sum_{x=1}^{V} h_x + A)}},$$

that is,

$$\rho_{\phi_V} = \frac{\mathrm{e}^{-\beta H_V^A}}{\mathrm{Tr}\,\mathrm{e}^{-\beta H_V^A}} \quad\text{and}\quad \rho_{\omega_V} = \frac{\mathrm{e}^{-\beta(H_V^A + A)}}{\mathrm{Tr}\,\mathrm{e}^{-\beta(H_V^A+A)}}.$$

Indeed, it follows easily that $\mathrm{Dom}(\ln\rho_{\phi_V}) = \mathrm{Dom}(\ln\rho_{\omega_V})$ and $A = \ln\rho_{\phi_V} - \ln\rho_{\omega_V}$ is bounded. The identity (2.9) with $\phi_V = \psi_V$ then yields

$$S(\phi_V\,\|\,\omega_V) = \beta\phi_V(A) - \ln\mathrm{Tr}\,\mathrm{e}^{\beta(\mu\mathcal{N}-\sum_{x=1}^{V} h_x + A)} + V\ln\mathrm{Tr}\,\mathrm{e}^{\beta(\mu n_1 - h_1)}. \tag{2.10}$$

The general case then follows from the lower semi continuity of the relative entropy [10]:

$$S(\phi_V\,\|\,\omega_V) \leq \liminf_{V\to\infty} S(\phi_{V,\epsilon}\,\|\,\omega_V).$$

Indeed, first assuming $\phi_V \leq \lambda\omega_V$ we can put $\phi_{V,\epsilon} = (1-\epsilon)\phi_V + \epsilon\omega_V$ to conclude that the theorem holds in this case. In the general case, we use the approximation $\rho_{\phi_{V,\epsilon}} = \frac{P_\epsilon\rho_{\phi_V}P_\epsilon}{\mathrm{Tr}[P_\epsilon\rho_{\phi_V}P_\epsilon]}$. □

It is proved in [10], Corollary 5.21, that

$$S(\phi\,\|\,\omega_1\otimes\omega_2) \geq S(\phi_1\,\|\,\omega_1) + S(\phi_2\,\|\,\omega_2). \tag{2.11}$$

The relative entropy is therefore superadditive:

$$S(\phi_{V1+V2}\,\|\,\omega_{V_1}\otimes\omega_{V_2}) \geq S(\phi_{V_1}\,\|\,\omega_{V_1}) + S(\phi_{V_2}\,\|\,\omega_{V_2}). \tag{2.12}$$

It follows that the mean entropy

$$s(\phi\,\|\,\omega) := \lim_{V\to\infty}\frac{1}{V}S(\phi_V\,\|\,\omega_V)$$

exists. We now have the following 'level-III' variational expression for the pressure. Here level-III refers to the fact that in the variational formula we optimise over states of the infinite system [7]. The set of all regular translation-invariant states on $\mathcal{A}$ is denoted by $\mathcal{S}(\mathcal{A})$, and the set of all regular translation-invariant and permutation-invariant states on $\mathcal{A}$ by $\mathcal{S}_\Pi(\mathcal{A})$.

Theorem 2.4.

$$
\begin{aligned}
p(\beta,\mu,\lambda) &:= \lim_{V\to\infty} \frac{1}{\beta V} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N}-H_V)} \\
&= \sup_{\substack{\phi\in\mathcal{S}_\Pi:\\ \phi(n_x)<+\infty}} \Big\{ \phi(a_1^*a_2) - \frac{1}{\beta} s(\phi\,\|\,\omega) \Big\} + \frac{1}{\beta} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n_1 - h_1)}.
\end{aligned}
$$

Here the supremum is taken over all regular translation- and permutation-invariant states ϕ on $\mathcal{A}$ such that $\phi(n_x) < +\infty$ for all $x \in \mathbb{N}$.

Proof. We denote

$$
v_V = \Big(\frac{1}{V}\sum_{x=1}^V a_x^*\Big)\Big(\frac{1}{V}\sum_{y=1}^V a_y\Big)
$$

and

$$
P_V = \frac{1}{\beta} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + V v_V)}
$$

so that

$$
p(\beta,\mu,\lambda) = \lim_{V\to\infty} \frac{1}{V} P_V.
$$

We approximate v_V using a cut-off, and call this bounded operator also v_V. By Theorem 2.3

$$
S(\phi_V\,\|\,\omega_V) \geq \beta V \phi_V(v_V) - \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu\mathcal{N} - \sum_{x=1}^V h_x + V v_V)} + V \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n_1 - h_1)}.
$$

This implies, using Lemma 2.1, that

$$
\begin{aligned}
\liminf_{V\to\infty} \frac{1}{V} P_V \geq \sup_{\phi\colon \phi(n_x)<+\infty} & \Big\{ \phi(a_1^*a_2) - \frac{1}{\beta} s(\phi\,\|\,\omega) \Big\} \\
&+ \frac{1}{\beta} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n_1 - h_1)}.
\end{aligned}
$$

To prove the converse we seek an approximate maximiser. This is standard. We let

$$
\tilde\psi_V = \psi_V \otimes \psi_V \otimes \dots
$$

be the infinite tensor product of states and define

$$
\bar\psi_V = \frac{1}{V} \sum_{j=1}^V \tilde\psi_V \circ \tau_{j-1},
$$

where τ_j is the translation over j. This is a permutation-invariant state. We estimate the expectation of the energy density:

$$\begin{aligned}\bar{\psi}_V(a_1^*a_2) &= \frac{1}{V}\sum_{k=1}^{V}\tilde{\psi}_V(a_k^*a_{k+1})\\ &= \frac{1}{V}\sum_{k=1}^{V-1}\psi_V(a_k^*a_{k+1}) + \frac{1}{V}\psi_V(a_V^*)\psi_V(a_1)\\ &= \frac{1}{V^2}\sum_{x=1}^{V}\sum_{y=1;\,y\neq x}^{V}\psi_V(a_x^*a_y) + \frac{1}{V}\psi_V(a_V^*)\psi_V(a_1)\\ &= \frac{1}{V^2}\sum_{x,y=1}^{V}\psi_V(a_x^*a_y) - \frac{1}{V}\psi_V(a_1^*a_1) + \frac{1}{V}|\psi_V(a_1)|^2.\end{aligned} \tag{2.13}$$

Lemma 2.1 and the Cauchy-Schwarz inequality $|\psi_V(a_1)|^2 \leq \psi_V(a_1^*a_1)$ then imply that

$$|\bar{\psi}_V(a_1^*a_2) - \psi_V(v_V)| \to 0 \text{ as } V \to \infty. \tag{2.14}$$

It is known that the entropy is convex in both arguments [10]. In particular, we have

$$s(\lambda\phi_1 + (1-\lambda)\phi_2 \,\|\, \omega) \leq \lambda s(\phi_1 \,\|\, \omega) + (1-\lambda)s(\phi_2 \,\|\, \omega).$$

On the other hand, by a simple approximation, we have

$$\begin{aligned}S(\lambda\phi_{1,V} + (1-\lambda)\phi_{2,V} \,\|\, \omega_V) = &-\lambda\langle\Phi_{1,V}|\ \ln\Delta_{\Phi_V,\Omega_V}\,|\Phi_{1,V}\rangle\\ &-(1-\lambda)\langle\Phi_{2,V}|\ \ln\Delta_{\Phi_V,\Omega_V}\,|\Phi_{2,V}\rangle,\end{aligned}$$

where $\phi_V = \lambda\phi_{1,V} + (1-\lambda)\phi_{2,V}$. Using the fact that $\pi(\rho_{\Omega_V})$ and $\pi'(\rho_{\phi_V})$ respectively $\pi'(\rho_{\phi_{1,V}}), \pi'(\rho_{\phi_{2,V}})$, commute and the operator monotonicity of the inverse and the logarithm, we have

$$\begin{aligned}\pi'(\rho_{\phi_V}) \geq \lambda\pi'(\rho_{\phi_{1,V}}) \quad &\Longrightarrow \quad \Delta_{\Omega_V,\Phi_V} \leq \lambda^{-1}\Delta_{\Omega_V,\Phi_{1,V}}\\ &\Longrightarrow \quad \ln\Delta_{\Omega_V,\Phi_V} \leq \ln\Delta_{\Omega_V,\Phi_{1,V}} - \ln\lambda.\end{aligned}$$

Of course, a similar inequality holds w.r.t. $\phi_{2,V}$. Therefore

$$\begin{aligned}S(\lambda\phi_{1,V} + (1-\lambda)\phi_{2,V} \,\|\, \omega_V) \geq \lambda S(\phi_{1,V} \,\|\, \omega_V) &+ (1-\lambda)S(\phi_{2,V} \,\|\, \omega_V)\\ &+ \lambda\ln\lambda + (1-\lambda)\ln(1-\lambda).\end{aligned}$$

In the limit, we find in combination with the convexity above, that the mean relative entropy is affine in the first variable:

$$s(\lambda\phi_1 + (1-\lambda)\phi_2 \,\|\, \omega) = \lambda s(\phi_1 \,\|\, \omega_V) + (1-\lambda)s(\phi_2 \,\|\, \omega). \tag{2.15}$$

Applying this to the state $\bar{\psi}_V$ we get

$$s(\bar{\psi}_V \,\|\, \omega) = \frac{1}{V}\sum_{k=1}^{V} s(\tilde{\psi}_V \circ \tau_{k-1} | \, \omega)$$

provided the right-hand side exists. However, by the translation-invariance of ω, the right-hand side can be written as

$$\begin{aligned}\frac{1}{V}\sum_{k=1}^{V} s(\tilde{\psi}_V \circ \tau_{k-1} \| \, \omega) &= \lim_{n\to\infty} \frac{1}{nV^2}\sum_{k=1}^{V} S((\psi_V)^{\otimes n} \circ \tau_{k-1} \| \, \omega_{nV}) \\ &= \lim_{n\to\infty} \frac{1}{nV} S((\psi_V)^{\otimes n} \, \| \, (\omega_V)^{\otimes n}) \\ &= \frac{1}{V} S(\psi_V \, \| \, \omega_V).\end{aligned}$$

We therefore have

$$\Big(\bar{\psi}_V(a_1^* a_2) - \frac{1}{\beta} s(\bar{\psi}_V \, \| \, \omega)\Big) - \Big(\psi_V(v_V) - \frac{1}{\beta V} S(\psi_V \, \| \, \omega_V)\Big) \to 0 \qquad (2.16)$$

as $V \to \infty$. On the other hand, by Theorem 2.3 as above (see Eq. (2.10)),

$$\begin{aligned} S(\psi_V \, \| \, \omega_V) &= \beta V \psi_V(v_V) - \ln \frac{\operatorname{Tr} \mathrm{e}^{\beta(\mu \mathcal{N} - \sum_{x=1}^{V} h_x + V v_V)}}{\operatorname{Tr} \mathrm{e}^{\beta V(\mu n_1 - h_1)}} \\ &= \beta \psi_V(v_V) - \beta P_V \beta V \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n_1 - h_1)}. \end{aligned} \qquad (2.17)$$

□

The variational expression for the pressure can now be simplified by decomposing the state ϕ into an integral of extremal permutation-invariant states:

Theorem 2.5.

$$p(\beta,\mu,\lambda) = \sup_{\substack{\sigma \in \mathcal{S}(\mathcal{A}_1): \\ \sigma(n_1) < +\infty}} \Big\{ |\sigma(a_1)|^2 - \frac{1}{\beta} S(\sigma \, \| \, \omega_1) \Big\} + \frac{1}{\beta} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n_1 - h_1)}, \qquad (2.18)$$

where the supremum is now taken over regular states σ of $\mathcal{A}_1$ such that $\sigma(n_1) < +\infty$.

Proof. The set of permutation invariant states $\mathcal{S}_\pi(\mathcal{A})$ is a convex compact set in the weak$*$-topology, and it is metrizable because $\mathcal{A}$ is separable. By Choquet's theorem [17], we can therefore decompose an arbitrary state ϕ into an integral

$$\phi = \int_{\operatorname{ext}(\mathcal{S}_\pi(\mathcal{A}))} \psi \, \mu(\mathrm{d}\psi)$$

over the extremal points of $\mathcal{S}_\pi(\mathcal{A})$. Here μ is a probability measure on $\operatorname{ext}(\mathcal{S}_\pi(\mathcal{A}))$. But, by Størmer's theorem [15], the extremal permutation invariant states are the product states

$$\psi_\sigma = \sigma \otimes \sigma \otimes \dots,$$

where σ is a state of $\mathcal{A}_1$. Thus,

$$\phi = \int_{\mathcal{S}(\mathcal{A}_1)} \psi_\sigma \, \mu(\mathrm{d}\sigma).$$

Moreover, since $\phi(n_x) < \infty$, we have that $\sigma(n_1) < \infty$ for μ-almost every σ. It follows that

$$\phi(a_1^* a_2) = \int \sigma(a_1^*)\sigma(a_1)\,\mu(\mathrm{d}\sigma) = \int |\sigma(a_1)|^2\,\mu(\mathrm{d}\sigma).$$

For the entropy term we use the following lemma [17, Lemma 9.7]:

Lemma 2.6. *Suppose that X is a compact convex subset of a locally convex topological vector space. Let $f\colon X \to \mathbb{R}$ be an affine, lower semi continuous function on X, and suppose that μ is a (Radon) probability measure on X, $x_0 = \int x\,\mu(dx)$. Then*

$$\int f(x)\,\mu(\mathrm{d}x) = f(x_0).$$

Since the relative entropy (and hence the mean relative entropy) is lower semi continuous and affine, the lemma applies and we have

$$s(\phi \,\|\, \omega) = \int s(\psi_\sigma \,\|\, \omega)\,\mu(\mathrm{d}\sigma).$$

However, since ω is also a product measure, $s(\psi_\sigma \,\|\, \omega) = S(\sigma \,\|\omega_1)$. The Theorem now follows. □

Remark 2.7. Notice that the subset of regular states is also closed in the set of all states on $\mathcal{A}$ by the Banach-Steinhaus theorem. Indeed, if ϕ_α is a net of regular states converging to ϕ in weak$*$-topology then $\phi_\alpha(W(tf))$ converges uniformly on compact sets $t \in [a,b]$, where $W(tf)$ is the Weyl operator for $f \in \mathbb{C}^V$.

In the following we write a instead of a_1 and n for n_1. Our variational expression for the pressure can be further reduced to

Theorem 2.8.

$$p(\beta,\mu,\lambda) = \sup_{z\in\mathbb{C}}\{|z|^2 - I(z)\} + \frac{1}{\beta}\ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n - h)}, \tag{2.19}$$

where the rate function $I(z)$ is given by

$$I(z) = \sup_{\nu\in\mathbb{C}}\Big\{\bar{\nu} z + \nu\bar{z} - \frac{1}{\beta}\ln\frac{\operatorname{Tr}\mathrm{e}^{\beta(\mu n - h + (\nu a^* + \bar{\nu} a))}}{\operatorname{Tr}\mathrm{e}^{\beta(\mu n - h)}}\Big\}. \tag{2.20}$$

To prove this, we first need a lemma:

Lemma 2.9. *Denote*

$$\tilde{p}(\nu) = \frac{1}{\beta}\ln\operatorname{Tr}\mathrm{e}^{\beta(\mu n - h + (\nu a^* + \bar{\nu} a))}. \tag{2.21}$$

This function is convex and satisfies

$$\tilde{p}(\nu) \sim |\nu|^{4/3} \text{ as } |\nu| \to \infty. \tag{2.22}$$

Proof of Lemma 2.9. Differentiating, we have

$$\tilde{p}'(\nu) = \langle a^* \rangle_{H(\nu)},$$

where

$$H(\nu) = -\mu n + h - \nu a^* - \bar{\nu} a.$$

Differentiating again, we get, as in [1], with $\nu = x + iy$,

$$\frac{\partial^2}{\partial x^2}\tilde{p}(\nu) = \Big(\frac{\partial}{\partial \nu} + \frac{\partial}{\partial \bar{\nu}}\Big)^2 \tilde{p}(\nu) = \beta\big(a + a^* - \langle a + a^* \rangle \,|\, a + a^* - \langle a + a^* \rangle\big)_{H(\nu)},$$

$$\frac{\partial^2}{\partial y^2}\tilde{p}(\nu) = -\Big(\frac{\partial}{\partial \nu} - \frac{\partial}{\partial \bar{\nu}}\Big)^2 \tilde{p}(\nu) = \beta\big(a - a^* - \langle a - a^* \rangle \,|\, a - a^* - \langle a - a^* \rangle\big)_{H(\nu)},$$

and

$$\begin{aligned}\frac{\partial^2}{\partial x \partial y}\tilde{p}(\nu) &= i\Big(\frac{\partial}{\partial \nu} + \frac{\partial}{\partial \bar{\nu}}\Big)\Big(\frac{\partial}{\partial \nu} - \frac{\partial}{\partial \bar{\nu}}\Big)\tilde{p}(\nu) \\ &= i\beta\big(a + a^* - \langle a + a^* \rangle \,|\, a^* - a - \langle a^* - a \rangle\big)_{H(\nu)}.\end{aligned}$$

It follows by the Cauchy-Schwarz inequality that the corresponding matrix is positive-definite.

To prove the asymptotic behaviour, we first remark that

$$\nu a^* + \bar{\nu} a \le 2|\nu|(n+1)^{1/2}$$

and hence

$$\begin{aligned}\tilde{p}(\nu) &\le \frac{1}{\beta} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n - h + 2|\nu|(n+1)^{1/2})} \\ &= \frac{1}{\beta} \ln \sum_{n=0}^{\infty} \mathrm{e}^{\beta((\mu-1)n - \lambda n(n-1) + 2|\nu|\sqrt{n+1})} = O(|\nu|^{4/3}).\end{aligned}$$

For the reverse inequality we use one half of the Berezin-Lieb bounds [18]:

$$\operatorname{Tr} \mathrm{e}^{-H(\nu)} \ge \int \frac{\mathrm{d}z\, \mathrm{d}\bar{z}}{\pi} \mathrm{e}^{-\langle z \,|\, H(\nu) \,|\, z \rangle}.$$

Here $|z\rangle$ stands for the coherent state

$$|z\rangle = \mathrm{e}^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n (a^*)^n}{n!} |0\rangle.$$

Since

$$\langle z|\, a \,|z\rangle = z, \qquad \langle z|\, a^* \,|z\rangle = \bar{z},$$
$$\langle z|\, n \,|z\rangle = |z|^2,$$

and

$$\langle z|\, (a^*)^2 a^2 \,|z\rangle = |z|^4,$$

we get

$$\operatorname{Tr} \mathrm{e}^{-H(\nu)} \ge \int \frac{\mathrm{d}z\, \mathrm{d}\bar{z}}{\pi}\, \mathrm{e}^{\beta((\mu-1)|z|^2 - \lambda |z|^4 + \bar{\nu} z + \nu \bar{z})} = O(|\nu|^{4/3}).$$

$\square$

Proof of Theorem 2.8. Take A to be an approximation of $\nu a^* + \bar{\nu} a$ in Theorem 2.3. We get, writing

$$p(\nu) = \frac{1}{\beta} \ln \operatorname{Tr} \mathrm{e}^{\beta(\mu n - h + (\nu a^* + \bar{\nu} a))},$$

the inequality

$$|\phi(a)|^2 - \frac{1}{\beta} S(\phi_V \,\|\, \omega_V) \leq |\phi(a)|^2 - \phi(\nu a^* + \bar{\nu} a) + p(\nu) - p(0)$$

and since ν is arbitrary,

$$|\phi(a)|^2 - \frac{1}{\beta} S(\phi \,\|\, \omega) \leq |\phi(a)|^2 - I(\phi(a)).$$

Conversely, suppose that z is a maximiser for $\sup\{|z|^2 - I(z)\}$. For any $\nu \in \mathbb{C}$, define the state ϕ_ν by

$$\rho_{\phi_\nu} = \frac{\mathrm{e}^{\beta(\mu n - h + (\nu a^* + \bar{\nu} a))}}{\operatorname{Tr} \mathrm{e}^{\beta(\mu n - h + (\nu a^* + \bar{\nu} a))}}$$

and choose ν such that $\phi_\nu(a) = z$. It follows from the above lemma that such ν exists. Then

$$\begin{aligned}
\sup_\phi \left\{ |\phi(a)|^2 - \frac{1}{\beta} S(\phi \,\|\, \omega) \right\} &\geq |\phi_\nu(a)|^2 - S(\phi_\nu \,||\, \omega) \\
&= |z|^2 - \phi_\nu(\nu a^* + \bar{\nu} a) + p(\nu) - p(0) \\
&= |z|^2 - I(z).
\end{aligned}$$

□

We finally rewrite the expression in the form (1.3). With a gauge transformation it is easy to see that $I(z)$ only depends on $|z|$ and we have

$$p(\beta, \mu, \lambda) = \sup_{x \geq 0} \left\{ x^2 - I(x) \right\} + p(0) \tag{2.23}$$

and

$$I(x) = \sup_{r \geq 0} \{2rx - p(r)\} + p(0). \tag{2.24}$$

Now let $r \geq 0$ be given, and suppose that $x_{\max}$ is a maximiser of the expression (2.23). Then

$$p(\beta, \mu, \lambda) = x_{\max}^2 - I(x_{\max}) + p(0) \leq x_{\max}^2 - 2r x_{\max} + p(r)$$

and choosing $r = x_{\max}$,

$$p(\beta, \mu, \lambda) \leq -x_{\max}^2 + p(x_{\max}) \leq \sup_{r \geq 0} \{-r^2 + p(r)\}.$$

On the other hand, if r_0 is a maximiser of the right-hand side, then

$$r_0 = \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}r} p(r) \big|_{r = r_0}$$

and hence

$$I(r_0) = 2r_0^2 - p(r_0) + p(0).$$

Inserting, we get

$$\sup_{r\geq 0}\{-r^2+p(r)\} = -r_0^2+p(r_0) = r_0^2 - I(r_0) + p(0) \leq p(\beta,\mu,\lambda).$$

Hence, we have shown the formula (1.3) for the infinite range Bose-Hubbard model (2.1).

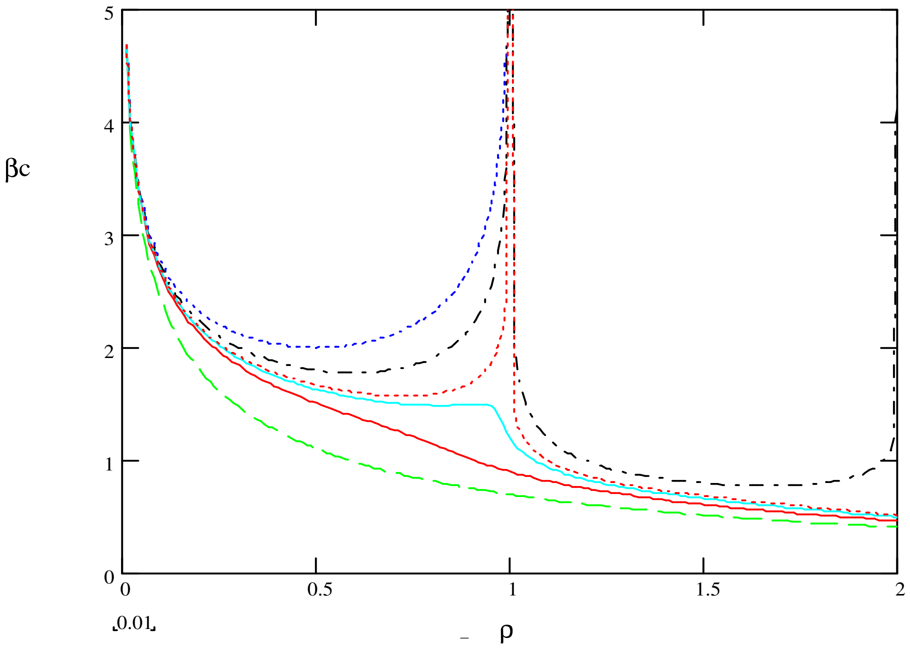
3. Analysis of the phase diagram

The phase diagram of the model was analysed in [1]. The same model, but with disorder, was analysed in [16] where it was found that the disorder gives rise to new phenomena. Unfortunately, [1] contains a few errors, which we wish to correct here. First of all, the critical values of lambda are not given by (2.14) of [1], but instead

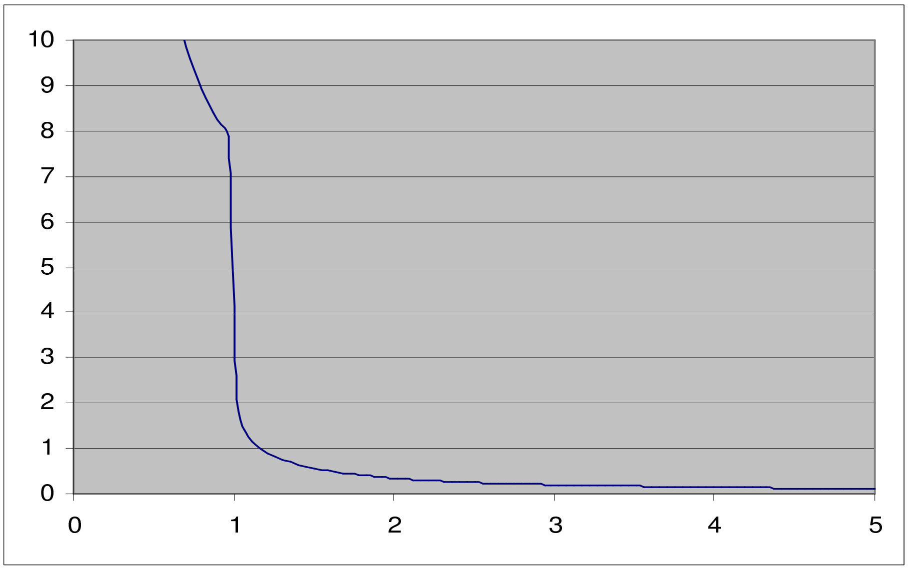
$$\lambda_{c,k} = 2k+1. \tag{3.1}$$

This was already remarked in [16], see Remark 4.1. Indeed, although a gap exists for $\lambda > \lambda_k$ given by (2.14) in [1], the limiting value of $\mu(\beta,\lambda)$ lies in this gap only if $\lambda > \lambda_{c,k}$.

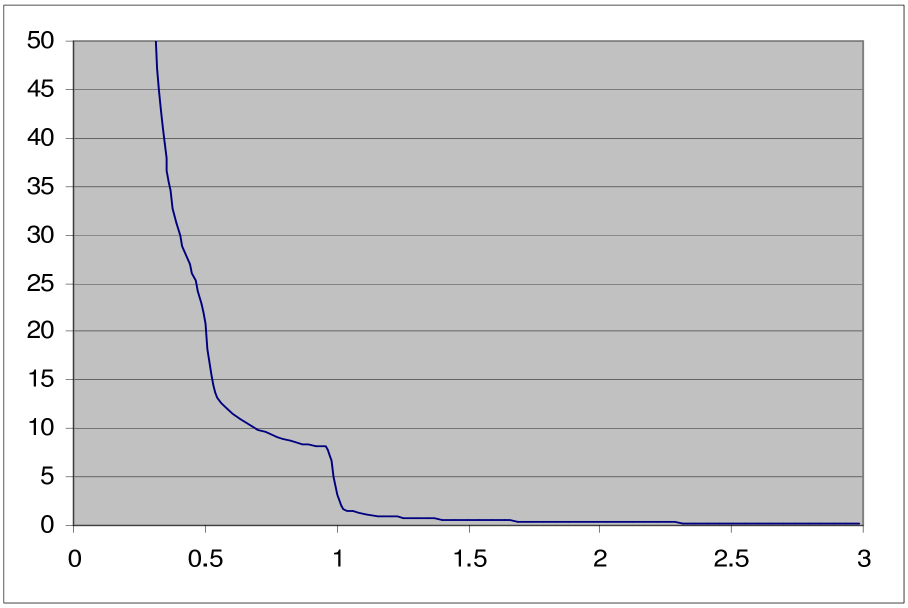
There was also a mistake in the program to compute the $p-V$ diagrams of Fig. 5 and 6 in [1], as well as the condensation fractions of Fig. 7 and 8. We include corrected graphs below:



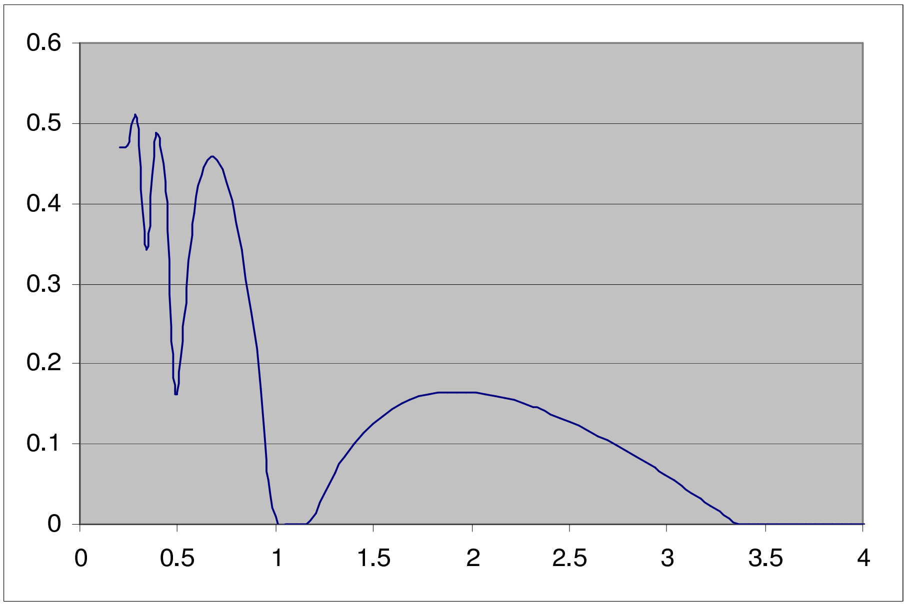
The critical inverse temperature as a function of the density for a number of values of λ.



The P-V diagram for $\lambda = 5$.



The P-V diagram for $\lambda = 5$ at higher pressures.



The condensation fraction as a function of the density for $\lambda = 5$.

4. The nearest-neighbour hopping model

As in the case of quantum spin models, there is also a variational formula for the pressure of the translation-invariant Bose-Hubbard model, analogous to Theorem 2.4:

Theorem 4.1. *The pressure of the nearest-neighbour hopping Bose-Hubbard model is given by*

$$\begin{aligned} p(\beta,\mu,\lambda) = \sup_{\phi:\,\phi(n_x)<+\infty} &\Big\{ \sum_{\nu=1}^{d} \phi(a_0^* a_{\mathrm{e}_\nu} + a_{\mathrm{e}_\nu}^* a_0) - \frac{1}{\beta} s(\phi \,\|\, \omega) \Big\} \\ &+ \frac{1}{\beta} \ln \mathrm{Tr}\, \mathrm{e}^{\beta(\mu \hat{n} - h_0)}, \end{aligned} \tag{4.1}$$

where the supremum is over all regular translation-invariant states ϕ on the CCR algebra such that $\phi(n_x) < +\infty$, and ω is the product state $\omega = \bigotimes_{x\in\mathbb{Z}^d} \omega_x$ with

$$\rho_{\omega_x} = \frac{1}{Z_0} \mathrm{e}^{\beta(\mu \hat{n}_x - h_x)}$$

and

$$h_x = d\,\hat{n}_x - \lambda \hat{n}_x(\hat{n}_x - 1).$$

The derivation of this formula is completely analogous to that of Theorem 2.4. The main difference is that the infinite-volume limit now has to taken in the sense of Van Hove. For the case of spin models, see for example [19] or [20]. This variational formula does not seem to have been written down before, though it has to be said that it is not clear how useful this formula is. The analogous formula for spin models has so far not been very useful for analysing the phase diagram. One possible application is perhaps the cluster variation approximation, see [21], [22], [23], [24].

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