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Long Cycles in the Infinite-Range-Hopping Bose-Hubbard Model with Hard Cores

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Abstract In this paper we study the relation between long cycles and Bose-Condensation in the Infinite range Bose-Hubbard Model with a hard core interaction. We calculate the density of particles on long cycles in the thermodynamic limit and find that the existence of a non-zero long cycle density coincides with the occurrence of Bose-Einstein condensation but this density is not equal to that of the Bose condensate.

Keywords Bose-Einstein Condensation · Cycles · Infinite range Bose-Hubbard Model

1 Introduction

In 1953, Feynman analysed the partition function of an interacting Bose gas in terms of the statistical distribution of permutation cycles of particles and emphasized the roles of long cycles at the transition point [6, 7]. Then Penrose and Onsager, pursuing Feynman's arguments, observed that there should be Bose condensation when the fraction of the total particle number belonging to long cycles is strictly positive [12]. These ideas are now commonly accepted and also discussed in various contexts in systems showing analogous phase transitions such as percolation, gelation and polymerization (see e.g. [4, 14, 15]), though it has been recently argued by Ueltschi [20] that in fact the hypothesis is not always valid. To our knowledge, there had not appeared a precise mathematical and quantitative formulation of the relation between Bose condensate and long cycles until the work of Sütö [16, 17] and its validity has been checked only in a few models: the free and mean field Bose gas in [16, 17], (see also Ueltschi [19]) and the perturbed mean field model of a Bose gas studied in [5]. In these models it is shown that the density of particles in long cycles is equal to the

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Bose condensate density. The purpose of this paper is test the validity of the hypothesis in yet another model of a Bose gas, the Infinite range Bose-Hubbard Model with a hard core. Here we calculate the density of particles on long cycles in the thermodynamic limit and find that though the existence of a non-zero long cycle density coincides with the occurrence of Bose-Einstein condensation, this density is not equal to the Bose condensate density.

The main simplifying feature in this model is the following. In general the density of particles on cycles of length q for n particles can be expressed (apart from normalization) as the trace (see for example Proposition 3.1) of the exponential of the Hamiltonian for $n-q$ bosons and q distinguishable particles (no statistics). In terms of the random walk representation (cf. [18]), the particles in this model are allowed to hop from one site to another with equal probability. We can prove (Proposition 3.2) that in the thermodynamic limit we can neglect the hopping of the q particles so that bosons have to avoid each other and the fixed positions of the distinguishable particles. This is equivalent to a reduction of the lattice by q sites. Moreover the q particles are on a cycle of length q. For $q>1$, this means for example, that the position of the second particle at the beginning of its path is same as the position of the first particle at the end of its path. But since they do not hop this is impossible by the hard core condition and therefore among the short cycles only the cycle of unit length contributes. Since the sum of all the cycle densities gives the particle density, this means that in the thermodynamic limit the sum of the long cycle densities is the particle density less the one-cycle contribution. The one-cycle density, apart from some scaling and the normalization, is then the partition function for the boson system with one site removed from the lattice, which can be calculated.

The model without a hard-core will be treated in another paper. There we can again neglect the hopping of the q distinguishable particles. However in that case cycles of all lengths contribute to the long-cycle density. It is relatively easy to see that when there is no condensation the long-cycle density vanishes but we do not yet know what happens when there is Bose-Einstein condensation.

In Sect. 2 we first describe the model and recall its thermodynamic properties as stated by Penrose [13] (see also Tóth [18] and Kirson [9]). We then apply the general framework for cycle statistics described in [5], following [11]. Using standard properties of the decomposition of permutations into cycles, the canonical sum is converted into a sum on cycle lengths. This makes it possible to decompose the total density $\rho = \rho_{\text{short}} + \rho_{\text{long}}$ into the number density of particles belonging to cycles of finite length (ρ_{short}) and to infinitely long cycles (ρ_{long}) in the thermodynamic limit. It is conjectured that when there is Bose condensation, ρ_{long} is different from zero and identical to the condensate density. The main purpose of the paper is to check the validity of this conjecture in our model. At the end of Sect. 2 we state in the main theorem describing the relation between Bose-Einstein condensation and the density of long cycles for our model.

In Sect. 3 we prove the main theorem and in Sect. 4 we discuss briefly *Off-diagonal Long-Range Order*.

2 The Model and Results

The Bose-Hubbard Hamiltonian is given by

$$H^{\text{BH}} = J \sum_{x,y\in\Lambda_V:|x-y|=1} (a_x^* - a_y^*)(a_x - a_y) + \lambda \sum_{x\in\Lambda_V} n_x(n_x - 1) \tag{2.1}$$

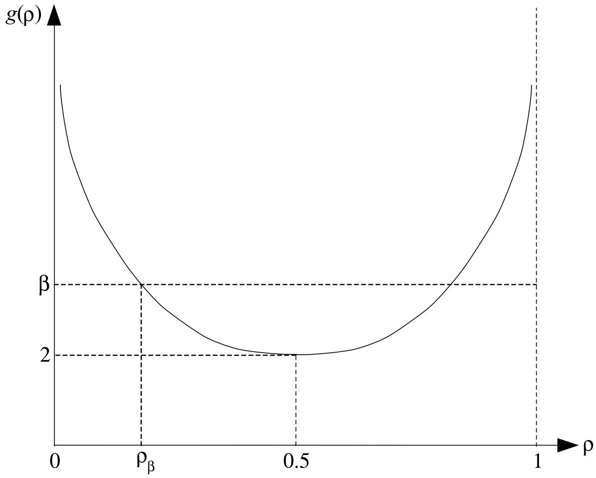


Fig. 1 Definition of ρ_β

where Λ_V is a lattice of V sites, a_x^* and a_x are the Bose creation and annihilation operators satisfying the usual commutation relations $[a_x^*, a_y] = \delta_{x,y}$ and $n_x = a_x^* a_x$. The first term with $J > 0$ is the kinetic energy operator and the second term with $\lambda > 0$ describes a repulsive interaction, as it discourages the presence of more than one particle at each site. This model was originally introduced by Fisher *et al.* [8].

The infinite-range hopping model is given by the Hamiltonian

$$H^{\mathrm{IR}} = \frac{1}{2V} \sum_{x,y \in \Lambda_V} (a_x^* - a_y^*)(a_x - a_y) + \lambda \sum_{x \in \Lambda_V} n_x(n_x - 1). \tag{2.2}$$

This is in fact a mean-field version of (2.1) 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, so we can take $\Lambda_V = \{1, 2, 3, \ldots, V\}$. The non-zero temperature properties of this model have been studied by Bru and Dorlas [3] and by Adams and Dorlas [1]. We shall study a special case of (2.2), introduced by Tóth [18] where $\lambda = +\infty$, that is complete single-site exclusion (hard-core). The properties of this model in the canonical ensemble were first obtained by Tóth using probabilistic methods. Later Penrose [13] and Kirson [9] obtained equivalent results. In the grand-canonical ensemble the model is equivalent to the strong-coupling BCS model (see for example Angelescu [2]). Here we recall the thermodynamic properties of the model in the canonical ensemble as given by Penrose.

For $\rho \in (0, 1)$, let

$$g(\rho) = \begin{cases} \dfrac{1}{1-2\rho} \ln\left(\dfrac{1-\rho}{\rho}\right) & \text{if } \rho \neq 1/2, \\ 2 & \text{if } \rho = 1/2. \end{cases}$$

For each $\beta \geq 2$ the equation $\beta = g(\rho)$ has a unique solution in $(0, 1/2]$ denoted by ρ_β (see Fig. 1). We define $\rho_\beta := 1/2$ for $\beta < 2$.

Theorem 2.1 (Penrose [13, Theorem 1]) *The free energy per site at inverse temperature β as a function of the particle density $\rho \in [0,1]$, $f_\beta(\rho)$, is given by*

$$f_\beta(\rho) = \begin{cases} \rho + \frac{1}{\beta}(\rho \ln \rho + (1-\rho)\ln(1-\rho)) & \text{if } \rho \in [0,\rho_\beta] \cup [1-\rho_\beta, 1], \\ \rho^2 + \rho_\beta(1-\rho_\beta) + \frac{1}{\beta}(\rho_\beta \ln \rho_\beta + (1-\rho_\beta)\ln(1-\rho_\beta)) & \text{if } \rho \in [\rho_\beta, 1-\rho_\beta]. \end{cases}$$

The density of particles in the ground state in the thermodynamic limit is given by

$$\rho_\beta^c = \lim_{\substack{n,V\to\infty \\ n/V=\rho}} \frac{1}{V^2} \sum_{x,y\in\Lambda_V} \langle a_x^* a_y \rangle \tag{2.3}$$

where $\langle \cdot \rangle$ denotes the canonical expectation for n particles. Penrose showed that for certain values of ρ and β, Bose-Einstein condensation occurs, that is, $\rho_\beta^c > 0$. The Bose-condensate density is given in the following theorem.

Theorem 2.2 (Penrose [13, Theorem 2]) *The Bose-condensate density, ρ_β^c at inverse temperature β as a function of the particle density $\rho \in [0,1]$, is given by*

$$\rho_\beta^c = \begin{cases} 0 & \text{if } \rho \in [0,\rho_\beta] \cup [1-\rho_\beta, 1], \\ (\rho-\rho_\beta)(1-\rho-\rho_\beta) & \text{if } \rho \in [\rho_\beta, 1-\rho_\beta]. \end{cases}$$

We note that both $f_\beta(\rho) - \rho$ and the condensate density ρ_β^c are symmetric about $\rho = 1/2$. This can easily seen by interchanging particles and holes. The Boson states being symmetric can be labelled unambiguously by the sites they occupy but equivalently they can be labelled by the sites they do not occupy (holes).

Before proceeding to the study of cycle statistics we need to define the n-particle Hamiltonian more carefully. The single particle Hilbert space is $\mathcal{H}_V := \mathbb{C}^V$ and on it we define the operator

$$H_V = I - P_V$$

where P_V is the orthogonal projection onto the unit vector

$$\mathbf{g}_V = \frac{1}{\sqrt{V}}(1,1,\dots,1) \in \mathcal{H}_V.$$

In terms of the usual basis vectors of $\mathcal{H}_V$, $\{\mathbf{e}_i \mid i = 1\dots V\}$, P_V is given by

$$P_V \mathbf{e}_i = \frac{1}{V}\sum_{j=1}^{V} \mathbf{e}_j.$$

Thus H_V is the orthogonal projection onto the subspace orthogonal to $\mathbf{g}_V$. For an operator A on $\mathcal{H}_V$, we define $A^{(n)}$ on $\mathcal{H}_V^{(n)} = \underbrace{\mathcal{H}_V \otimes \mathcal{H}_V \otimes \cdots \otimes \mathcal{H}_V}_{n \text{ times}}$ by

$$A^{(n)} = A \otimes I \otimes \cdots \otimes I + I \otimes A \otimes \cdots \otimes I + \cdots + I \otimes I \otimes \cdots \otimes A.$$

With this notation we can define the non-interacting n-particle Hamiltonian $H_V^{(n)}$ acting on the unsymmetrised Hilbert space $\mathcal{H}_V^{(n)}$ as:

$$H_V^{(n)} = I^{(n)} - P_V^{(n)}$$

$$= n - P_V \otimes I \otimes \cdots \otimes I - I \otimes P_V \otimes I \otimes \cdots \otimes I - \cdots - I \otimes I \otimes \cdots \otimes P_V.$$

For bosons we have to consider the symmetric subspace of $\mathcal{H}_V^{(n)}$. The symmetrisation projection σ_+^n on $\mathcal{H}_V^{(n)}$ is defined by

$$\sigma_+^n = \frac{1}{n!} \sum_{\pi \in S_n} U_\pi \tag{2.4}$$

where $U_\pi : \mathcal{H}_V^{(n)} \mapsto \mathcal{H}_V^{(n)}$ is the unitary representation of the permutation group S_n on $\mathcal{H}_V^{(n)}$ defined by

$$U_\pi(\phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n) = \phi_{\pi(1)} \otimes \phi_{\pi(2)} \otimes \cdots \otimes \phi_{\pi(n)}, \quad \phi_j \in \mathcal{H}_V, \quad j = 1, \ldots, n; \ \pi \in S_n.$$

Then the symmetric n-particle subspace is $\mathcal{H}_{V,+}^{(n)} := \sigma_+^n \mathcal{H}_V^{(n)}$.

When $H_V^{(n)}$ is restricted to $\mathcal{H}_{V,+}^{(n)}$, we obtain

$$\frac{1}{2V} \sum_{x,y \in \Lambda_V} (a_x^* - a_y^*)(a_x - a_y).$$

We introduce the hard-core interaction by applying a projection to $\mathcal{H}_V^{(n)}$ to forbid more than one particle from occupying each site. Let $\{\mathbf{e}_i\}_{i=1}^V$ be the usual orthonormal basis for $\mathcal{H}_V$. We then define the hard core projection $\mathcal{P}_n^{\mathsf{hc}}$ on $\mathcal{H}_V^{(n)}$ by

$$\mathcal{P}_n^{\mathsf{hc}}(\mathbf{e}_{i_1} \otimes \mathbf{e}_{i_2} \otimes \cdots \otimes \mathbf{e}_{i_n}) = \begin{cases} 0 & \text{if } i_k = i_{k'} \ \text{ for some } k \neq k', \\ \mathbf{e}_{i_1} \otimes \mathbf{e}_{i_2} \otimes \cdots \otimes \mathbf{e}_{i_n} & \text{otherwise.} \end{cases} \tag{2.5}$$

We shall call $\mathcal{H}_{n,V}^{\mathsf{hc}} := \mathcal{P}_n^{\mathsf{hc}} \mathcal{H}_V^{(n)}$ the unsymmetrised hard-core n-particle space and $\mathcal{H}_{n,V,+}^{\mathsf{hc}} := \mathcal{P}_n^{\mathsf{hc}} \mathcal{H}_{V,+}^{(n)}$ the symmetric hard-core n-particle space. Note that as $[U_\pi, \mathcal{P}_n^{\mathsf{hc}}] = 0$ for all $\pi \in S_n$, $\mathcal{P}_n^{\mathsf{hc}}$ commutes with the symmetrisation and so $\mathcal{H}_{n,V,+}^{\mathsf{hc}} = \sigma_+^n \mathcal{H}_{n,V}^{\mathsf{hc}}$.

The hard-core n-particle Hamiltonian is then

$$H_{n,V}^{\mathsf{hc}} := \mathcal{P}_n^{\mathsf{hc}} H_V^{(n)} \mathcal{P}_n^{\mathsf{hc}} \tag{2.6}$$

acting on the hard-core n-particle space $\mathcal{H}_{n,V}^{\mathsf{hc}}$. Therefore the Hamiltonian for the infinite-range Bose-Hubbard model with hard-core is (2.6) acting on the **symmetric** hard-core n-particle space $\mathcal{H}_{n,V,+}^{\mathsf{hc}}$.

We shall now analyse the cycle statistics of this model.

Using (2.4), the canonical partition function for the hard-core boson model may be written as

$$Z_\beta(n, V) = \operatorname{trace}_{\mathcal{H}_{n,V,+}^{\mathsf{hc}}}\left[\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right] = \operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[\sigma_+^n \mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right] = \frac{1}{n!} \sum_{\pi \in S_n} \operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[U_\pi \mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right].$$

Following [5], we define a probability measure on the permutation group S_n by

$$\mathbb{P}_V^n(\pi) = \frac{1}{Z_\beta(n, V)} \frac{1}{n!} \operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[U_\pi \mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right]. \tag{2.7}$$

From the random walk formulation (see for example [18]) one can see that the kernel of $\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}$ is positive and therefore the righthand side of (2.7) is positive.

Each permutation $\pi \in S_n$ can be decomposed uniquely into a number of cyclic permutations of lengths $q_1, q_2, \ldots, q_r$ with $r \le n$ and $q_1 + q_2 + \cdots + q_r = n$. For $q \in \{1, 2, \ldots, n\}$, let $N_q(\pi)$ be the random variable corresponding to the number of cycles of length q in π. Then the expectation of the number of q-cycles in the canonical ensemble is:

$$\mathbb{E}_V^n(N_q) = \sum_{r=1}^{n} r \mathbb{P}_V^n(N_q = r)$$

and the average density of particles in q-cycles for the system of n bosons is

$$c_V^n(q) = \frac{q\, \mathbb{E}_V^n(N_q)}{V}. \tag{2.8}$$

This brings us then to the following definition.

Definition 1 The expected density of particles on cycles of **infinite** length is given by

$$\rho_\beta^{\text{long}} = \lim_{Q\to\infty} \lim_{\substack{n,V\to\infty \\ n/V=\rho}} \sum_{q=Q+1}^{n} c_V^n(q). \tag{2.9}$$

For the free Bose gas, the mean field and the perturbed mean field Bose gas, it has been shown that $\rho_\beta^{\text{long}} = \rho_\beta^c$, the condensate density. For our model, the situation is different. Below we state the main result of this paper:

Theorem 2.3 *The expected density of particles on cycles of infinite length, ρ_β^{long}, at inverse temperature β as a function of the particle density $\rho \in [0, 1]$, is given by*

$$\rho_\beta^{\text{long}} = \begin{cases} 0 & \text{if } \rho \in [0, \rho_\beta] \cup [1-\rho_\beta, 1], \\ \rho - \rho_\beta e^{\beta(\rho-\rho_\beta)} & \text{if } \rho \in [\rho_\beta, 1-\rho_\beta]. \end{cases}$$

We note that (see Fig. 2):

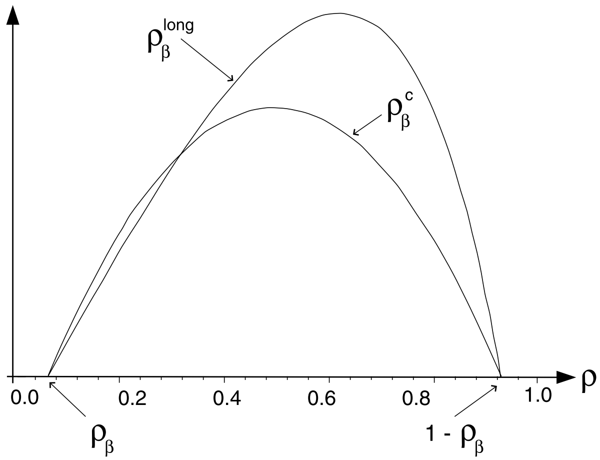
- $\rho_\beta^{\text{long}} = 0$ if and only if $\rho_\beta^c = 0$.
- ρ_β^{long} is not symmetric with respect to $\rho = 1/2$. As mentioned above the symmetry of the model about $\rho = 1/2$ is due to the particle-hole symmetry. But the equivalent labelling of states by sets of occupied or unoccupied sites (particles and holes) cannot be used for distinguishable particles. We shall see (Proposition 3.1) that the q-cycle occupation density $c_V^n(q)$ involves q distinguishable particles and $n-q$ bosons and therefore the particle-hole symmetry is broken.
- When $\rho_\beta^c > 0$, ρ_β^{long} starts below ρ_β^c since its slope at ρ_β is equal to $1 - 2\rho_\beta$ while ρ_β^c has slope $1 - \beta\rho_\beta$ and $\beta > 2$. Conversely, ρ_β^{long} finishes above ρ_β^c since its slope at $1-\rho_\beta$ is less than that of ρ_β^c.

3 Proof of the Main Result

In this section we shall prove Theorem 2.3. First we note that if $n/V = \rho$, then

$$\sum_{q=1}^{n} c_V^n(q) = \rho, \tag{3.1}$$

Fig. 2 ρ_β^c and ρ_β^{long} for $\beta > 2$



so that if we define

$$\rho_\beta^{\text{short}} = \lim_{Q\to\infty} \lim_{\substack{n,V\to\infty\\ n/V=\rho}} \sum_{q=1}^{Q} c_V^n(q)$$

we have

$$\rho_\beta^{\text{long}} = \rho - \rho_\beta^{\text{short}}.$$

For $\rho_\beta^{\text{short}}$ we can interchange the sum over q and $\lim_{\substack{n,V\to\infty\\ n/V=\rho}}$,

$$\rho_\beta^{\text{short}} = \lim_{Q\to\infty} \sum_{q=1}^{Q} \lim_{\substack{n,V\to\infty\\ n/V=\rho}} c_V^n(q),$$

making it much easier to calculate. In fact we shall prove that:

$$\rho_\beta^{\text{short}} = \begin{cases} \rho & \text{if } \rho \in [0,\rho_\beta] \cup [1-\rho_\beta, 1], \\ \rho_\beta e^{\beta(\rho-\rho_\beta)} & \text{if } \rho \in [\rho_\beta, 1-\rho_\beta]. \end{cases} \tag{3.2}$$

The proof is in four steps. The first step is to obtain a convenient expression for $c_V^n(q)$, the mean density of particles belonging to a cycle of length q. We shall denote the unitary representation of a q-cycle by $U_q : \mathcal{H}_V^{(q)} \to \mathcal{H}_V^{(q)}$, that is

$$U_q(\phi_1 \otimes \cdots \otimes \phi_n) = \phi_2 \otimes \cdots \phi_q \otimes \phi_1.$$

When there is no ambiguity we shall use the same notation U_q for $U_q \otimes I^{(n-q)} : \mathcal{H}_V^{(n)} \to \mathcal{H}_V^{(n)}$ where I is the identity operator. Note that $[U_q, \mathcal{P}_n^{\text{hc}}] = 0$ and $[U_q, \sigma_+^n] = 0$.

Proposition 3.1

$$c_V^n(q) = \frac{1}{Z_\beta(n,V)} \frac{1}{V} \operatorname{trace}_{\mathcal{H}_{q,n,V}^{\text{hc}}} \left[U_q e^{-\beta H_{n,V}^{\text{hc}}}\right]$$

where $\mathcal{H}_{q,n,V}^{\text{hc}} := \mathcal{P}_n^{\text{hc}}(\mathcal{H}_V^{(q)} \otimes \mathcal{H}_{V,+}^{(n-q)})$.

Note that though we write this proposition for our special case, in fact $c_V^n(q)$ can be expressed in this form for any Boson model with a symmetric Hamiltonian.

By using cycle statistics, we split our symmetric hard-core Hilbert space $\mathcal{H}_{n,V,+}^{\mathsf{hc}}$ into a tensor product of two spaces, an unsymmetrised q-particle space $\mathcal{H}_V^{(q)}$ and a symmetric $n-q$ particle space $\mathcal{H}_{V,+}^{(n-q)}$, with the hard-core projection applied. Writing

$$A^{(q)} := A^{(q)} \otimes I^{(n-q)} \quad \text{and} \quad A^{(n-q)} := I^{(q)} \otimes A^{(n-q)}$$

for any operator A on $\mathcal{H}_V$, we can express our Hamiltonian (2.6) on $\mathcal{H}_{q,n,V}^{\mathsf{hc}}$ as follows:

$$H_{n,V}^{\mathsf{hc}} = \mathcal{P}_n^{\mathsf{hc}}(n - P_V^{(q)} - P_V^{(n-q)})\mathcal{P}_n^{\mathsf{hc}}.$$

Let $\widetilde{P}_V^{(q)} = \mathcal{P}_n^{\mathsf{hc}} P_V^{(q)} \mathcal{P}_n^{\mathsf{hc}}$ and define the following reduced Hamiltonian

$$\widetilde{H}_{q,n,V}^{\mathsf{hc}} = \mathcal{P}_n^{\mathsf{hc}}(n - P_V^{(n-q)})\mathcal{P}_n^{\mathsf{hc}}, \tag{3.3}$$

so that

$$H_{n,V}^{\mathsf{hc}} = \widetilde{H}_{q,n,V}^{\mathsf{hc}} - \widetilde{P}_V^{(q)}.$$

The next step is to estimate the effect of neglecting the action of the $\widetilde{P}_V^{(q)}$ term (equivalent to the hopping of the q particles) in the unsymmetrised space. Let

$$\widetilde{c}_V^{\,n}(q) = \frac{1}{Z_\beta(n,V)} \frac{1}{V} \mathrm{trace}_{\mathcal{H}_{q,n,V}^{\mathsf{hc}}}\big[U_q \mathrm{e}^{-\beta \widetilde{H}_{q,n,V}^{\mathsf{hc}}}\big], \tag{3.4}$$

and define

$$Z_\beta(\lambda, n, V) = \mathrm{trace}_{\mathcal{H}_{n,V,+}^{\mathsf{hc}}}\big[\mathrm{e}^{-\beta H_{\lambda,n,V}^{\mathsf{hc}}}\big]$$

where

$$H_{\lambda,n,V}^{\mathsf{hc}} = \mathcal{P}_n^{\mathsf{hc}}(n - \lambda P_V^{(n)})\mathcal{P}_n^{\mathsf{hc}}. \tag{3.5}$$

Then we have the following estimate.

Proposition 3.2

$$|c_V^{\,n}(q) - \widetilde{c}_V^{\,n}(q)| \le \frac{(1 - \mathrm{e}^{-\beta q})}{V} \frac{Z_\beta(\frac{V-q}{V}, n-q, V-q)}{Z_\beta(n,V)}.$$

In the third step we obtain the limit of the ratio on the righthand side of the last inequality:

Proposition 3.3

$$\lim_{\substack{n,V\to\infty \\ n/V=\rho}} \frac{Z_\beta(\frac{V-q}{V}, n-q, V-q)}{Z_\beta(n,V)} = \begin{cases} \rho^q\, \mathrm{e}^{\beta q} & \text{if } \rho \in [0,\rho_\beta] \cup [1-\rho_\beta, 1], \\ \rho_\beta^q\, \mathrm{e}^{\beta q(1+\rho-\rho_\beta)} & \text{if } \rho \in [\rho_\beta, 1-\rho_\beta]. \end{cases} \tag{3.6}$$

The final step is a simple proposition where we check the following:

Proposition 3.4 $\widetilde{c}_V^n(q)=0$ *if* $q>1$ *and*

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}} \widetilde{c}_V^n(1)=\begin{cases}\rho & \text{if } \rho\in[0,\rho_\beta]\cup[1-\rho_\beta,1],\\ \rho_\beta\,\mathrm{e}^{\beta(\rho-\rho_\beta)} & \text{if } \rho\in[\rho_\beta,1-\rho_\beta].\end{cases} \tag{3.7}$$

Using these four results the main result, Theorem 2.3 follows very easily. From Propositions 3.2 and 3.3 we have

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}} c_V^n(q)=\lim_{\substack{n,V\to\infty\\ n/V=\rho}} \widetilde{c}_V^n(q).$$

Since by Proposition 3.4, $\widetilde{c}_V^n(q)=0$ if $q>1$, it follows that

$$\rho_\beta^{\text{short}}=\lim_{\substack{n,V\to\infty\\ n/V=\rho}} c_V^n(1)=\begin{cases}\rho & \text{if } \rho\in[0,\rho_\beta]\cup[1-\rho_\beta,1],\\ \rho_\beta\mathrm{e}^{\beta(\rho-\rho_\beta)} & \text{if } \rho\in[\rho_\beta,1-\rho_\beta]\end{cases}$$

which is the required result.

In the next four subsections we prove the results stated above.

3.1 Proof of Proposition 3.1

We recall the following facts on the permutation group.

- The decomposition into cycles leads to a partition of S_n into equivalence classes of permutations with the same cycle structure $C_{\mathbf{q}}$, where $\mathbf{q}=[q_1,q_2,\dots,q_r]$ is an unordered r-tuple of natural numbers with $q_1+q_2+\cdots+q_r=n$.
- Two permutation π' and π'' belong to the same class if and only if they are conjugate in S_n, i.e. if there exists a $\pi\in S_n$ such that

$$\pi''=\pi^{-1}\pi'\pi. \tag{3.8}$$

- The number of permutations belonging to the class $C_{\mathbf{q}}$ is

$$\frac{n!}{n_{\mathbf{q}}!(q_1q_2\cdots q_r)} \tag{3.9}$$

  with $n_{\mathbf{q}}!=n_1!n_2!\cdots n_j!\cdots$ and n_j is the number of cycles of length j in $\mathbf{q}$.

We observe that since our Hamiltonian is symmetric ($[H_{n,V}^{\mathsf{hc}},U_\pi]=0,\pi\in S_n$) and therefore for $\pi',\pi''\in C_{\mathbf{q}}$, one has by (3.8)

$$\begin{aligned}\operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}[U_{\pi''}\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}]&=\operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\big[U_\pi^{-1}U_{\pi'}U_\pi\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\big]\\ &=\operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\big[U_\pi^{-1}U_{\pi'}\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}U_\pi\big]\\ &=\operatorname{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\big[U_{\pi'}\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\big].\end{aligned} \tag{3.10}$$

For $q\in\mathbb{N}$, let $N_q(\pi)$ be the number of cycles of length q in π.

Let r_j denote the number of cycles of length j. Then $\sum_j jr_j=n$ and the corresponding number of permutations this cycle structure is $n!/\prod_j j^{r_j}r_j!$ (from (3.9)). Denote (r_j) the class of permutations with such a cycle structure. Then

$$\begin{aligned}\mathbb{P}_V^n(N_q=r)&=\frac{1}{Z_\beta(n,V)}\frac{1}{n!}\sum_{\substack{(r_j)\\ r_q=r}}\sum_{\pi\in(r_j)}\mathrm{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[U_\pi \mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right]\\&=\frac{1}{Z_\beta(n,V)}\frac{1}{n!}\sum_{\substack{(r_j)\\ r_q=r}}\frac{n!}{\prod_{j\ge 1}j^{r_j}r_j!}\mathrm{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[U_{\tilde\pi}\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right]\end{aligned}$$

where $\tilde\pi$ is any permutation with cycle distribution (r_j). Suppose that $r\ge 1$ and consider a permutation where the first q indices belong to the same cycle of length q. Let π' denote the permutation of the remaining $n-q$ indices. We have

$$U_\pi=U_q\otimes U_{\pi'}$$

and π' has cycle structure $(r_j-\delta_{jq})$. Then

$$\begin{aligned}&\mathbb{P}_V^n(N_q=r)\\&\quad=\frac{1}{Z_\beta(n,V)}\frac{1}{n!}\sum_{\substack{(r_j),\sum jr_j=n-q\\ r_q=r-1}}\frac{(n-q)!}{\prod_{j\ge 1}j^{r_j}r_j!}\frac{n!}{qr(n-q)!}\mathrm{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right]\\&\quad=\frac{1}{Z_\beta(n,V)}\frac{1}{qr(n-q)!}\sum_{\pi'\in S_{n-q}}\mathrm{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right].\end{aligned}$$

Then the canonical expectation of the number of q-cycles is found to be

$$\begin{aligned}\mathbb{E}_V^n(N_q)&=\sum_{r=0}^{\infty}r\mathbb{P}_V^n(N_q=r)\\&=\frac{1}{Z_\beta(n,V)}\frac{1}{q(n-q)!}\sum_{\pi'\in S_{n-q}}\mathrm{trace}_{\mathcal{H}_{n,V}^{\mathsf{hc}}}\left[(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right]\\&=\frac{1}{Z_\beta(n,V)}\frac{1}{q(n-q)!}\sum_{\pi'\in S_{n-q}}\mathrm{trace}_{\mathcal{H}_V^{(n)}}\left[\mathcal{P}_n^{\mathsf{hc}}(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\mathcal{P}_n^{\mathsf{hc}}\right]\\&=\frac{1}{Z_\beta(n,V)}\frac{1}{q}\mathrm{trace}_{\mathcal{H}_V^{(q)}\otimes\mathcal{H}_{V,+}^{(n-q)}}\left[\mathcal{P}_n^{\mathsf{hc}}(U_q\otimes I^{(n-q)})\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\mathcal{P}_n^{\mathsf{hc}}\right]\\&=\frac{1}{Z_\beta(n,V)}\frac{1}{q}\mathrm{trace}_{\mathcal{P}_n^{\mathsf{hc}}(\mathcal{H}_V^{(q)}\otimes\mathcal{H}_{V,+}^{(n-q)})}\left[(U_q\otimes I^{(n-q)})\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\right].\end{aligned}$$

Since

$$c_V^n(q)=\frac{q\,\mathbb{E}_V^n(N_q)}{V}$$

we have proved Proposition 3.1.

3.2 Proof of Proposition 3.2

To prove Proposition 3.2 we have to obtain an upper bound for

$$\left|\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}\left[U_q \mathrm{e}^{-\beta H^{\mathrm{hc}}_{n,V}}\right] - \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}\left[U_q \mathrm{e}^{-\beta \widetilde{H}^{\mathrm{hc}}_{q,n,V}}\right]\right|$$

In order to do this we first shall introduce some notation and make some remarks before proceeding.

Let $\Lambda^{(n-q)}_{V+}$ be the family of sets of $n-q$ distinct points of Λ_V. For $\mathbf{k} = \{k_1, k_2, \ldots, k_{n-q}\} \in \Lambda^{(n-q)}_{V+}$ let

$$|\mathbf{k}\rangle := \sigma^{n-q}_{+}(\mathbf{e}_{k_1} \otimes \mathbf{e}_{k_2} \otimes \cdots \otimes \mathbf{e}_{k_{n-q}}).$$

Then $\{|\mathbf{k}\rangle \mid \mathbf{k} \in \Lambda^{(n-q)}_{V+}\}$ is an orthonormal basis for $\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+} := \mathcal{P}^{\mathrm{hc}}_{n-q}\mathcal{H}^{(n-q)}_{V+}$.

Similarly let $\Lambda^{(q)}_V$ be the set of ordered q-tuples of distinct indices of Λ_V and for $\mathbf{i} = (i_1, i_2, \ldots, i_q) \in \Lambda^{(q)}_V$ let

$$|\mathbf{i}\rangle := \mathbf{e}_{i_1} \otimes \mathbf{e}_{i_2} \otimes \cdots \otimes \mathbf{e}_{i_q}.$$

Then $\{|\mathbf{i}\rangle \mid \mathbf{i} \in \Lambda^{(q)}_V\}$ is an orthonormal basis for $\mathcal{H}^{\mathrm{hc}}_{q,V} := \mathcal{P}^{\mathrm{hc}}_q\mathcal{H}^{(q)}_V$.

If $\mathbf{k} \in \Lambda^{(n-q)}_{V+}$ and $\mathbf{i} \in \Lambda^{(q)}_V$ we shall write $\mathbf{k} \sim \mathbf{i}$ if $\{k_1, k_2, \ldots, k_{n-q}\} \cap \{i_1, i_2, \ldots, i_q\} = \emptyset$ and we shall use the notation

$$|\mathbf{i}; \mathbf{k}\rangle := |\mathbf{i}\rangle \otimes |\mathbf{k}\rangle.$$

Then a basis for $\mathcal{H}^{\mathrm{hc}}_{q,n,V}$ may be formed by taking the tensor product of the bases of $\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}$ and $\mathcal{H}^{\mathrm{hc}}_{q,V}$ where we disallow particles from appearing in both spaces simultaneously. Thus the set $\{|\mathbf{i}; \mathbf{k}\rangle \mid \mathbf{k} \in \Lambda^{(n-q)}_{V+},\ \mathbf{i} \in \Lambda^{(q)}_V,\ \mathbf{k} \sim \mathbf{i}\}$ is an orthonormal basis for $\mathcal{H}^{\mathrm{hc}}_{q,n,V}$.

We shall need also the following facts. For simplicity we shall write $\widetilde{H}$ and $\widetilde{P}$ for $\widetilde{H}^{\mathrm{hc}}_{q,n,V}$ and $\widetilde{P}^{(q)}_V$ respectively, as defined in (3.3).

Let $\mathcal{P}^{(n-q)}_{\mathbf{i}}$ be the projection of $\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}$ onto a space with none of the $n-q$ particles at the points $i_1, i_2, \ldots, i_q$ (so there are $V-q$ available sites for $n-q$ particles) and not more than one particle at any site. Then

Remark 3.1 For $\mathbf{i} \sim \mathbf{k}$, if $s > 0$

$$\mathrm{e}^{-\beta\widetilde{H}s}|\mathbf{i}; \mathbf{k}\rangle = |\mathbf{i}; \mathrm{e}^{-\beta H^{\mathbf{i}}s}\mathbf{k}\rangle \mathrm{e}^{-\beta q s} \tag{3.11}$$

where $H^{\mathbf{i}} = \mathcal{P}^{(n-q)}_{\mathbf{i}}((n-q) - P^{(n-q)}_V)\mathcal{P}^{(n-q)}_{\mathbf{i}}$.

This can be seen as follows: For $\mathbf{i} \sim \mathbf{k}$,

$$\begin{aligned}
\widetilde{H}|\mathbf{i}; \mathbf{k}\rangle &= \mathcal{P}^{\mathrm{hc}}_n(n - P^{(n-q)}_V)\mathcal{P}^{\mathrm{hc}}_n|\mathbf{i}; \mathbf{k}\rangle \\
&= q\mathcal{P}^{\mathrm{hc}}_n|\mathbf{i}; \mathbf{k}\rangle + \mathcal{P}^{\mathrm{hc}}_n|\mathbf{i}; ((n-q) - P^{(n-q)}_V)\mathbf{k}\rangle \\
&= q|\mathbf{i}; \mathbf{k}\rangle + |\mathbf{i}; \mathcal{P}^{(n-q)}_{\mathbf{i}}((n-q) - P^{(n-q)}_V)\mathbf{k}\rangle \\
&= q|\mathbf{i}; \mathbf{k}\rangle + |\mathbf{i}; H^{\mathbf{i}}\mathbf{k}\rangle.
\end{aligned}$$

Remark 3.2 For $\mathbf{i}\sim\mathbf{k}$,

$$H^{\mathbf{i}}|\mathbf{k}\rangle=(n-q)|\mathbf{k}\rangle-\frac{1}{V}\sum_{l=1}^{n-q}\sum_{j\notin\mathbf{i}\cup\mathbf{k}\setminus\{k_l\}}|(k_1,k_2,\dots,\widehat{k_l},j,\dots,k_{n-q})\rangle \tag{3.12}$$

where the hat symbol implies the term is removed from the sequence, while from (3.5), for $\mathbf{k}\in\mathcal{H}_{V-q,+}^{(n-q)}$ we have

$$H^{\mathsf{hc}}_{\lambda,n-q,V-q}|\mathbf{k}\rangle=(n-q)|\mathbf{k}\rangle-\frac{\lambda}{V-q}\sum_{l=1}^{n-q}\sum_{\substack{j=1\\ j\notin\mathbf{k}\setminus\{k_l\}}}^{V-q}|(k_1,k_2,\dots,\widehat{k_l},j,\dots,k_{n-q})\rangle. \tag{3.13}$$

Thus $H^{\mathbf{i}}$ is unitarily equivalent to $H^{\mathsf{hc}}_{(V-q)/V,n-q,V-q}$ and

$$\operatorname{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\left[\mathcal{P}^{(n-q)}_{\mathbf{i}}\mathrm{e}^{-\beta\widetilde{H}^{\mathbf{i}}}\mathcal{P}^{(n-q)}_{\mathbf{i}}\right]=Z_\beta((V-q)/V,n-q,V-q). \tag{3.14}$$

Remark 3.3 For $s,\alpha\in\mathbb{R}$

$$\left(\mathcal{P}^{(n-q)}_{\mathbf{i}}\mathrm{e}^{-s\widetilde{H}^{\mathbf{i}}}\mathcal{P}^{(n-q)}_{\mathbf{i}}\right)^{\alpha}=\mathcal{P}^{(n-q)}_{\mathbf{i}}\mathrm{e}^{-s\alpha\widetilde{H}^{\mathbf{i}}}\mathcal{P}^{(n-q)}_{\mathbf{i}}.$$

We expand

$$\operatorname{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\left[U_q\mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]=\operatorname{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\left[U_q\mathrm{e}^{-\beta(\widetilde{H}-\widetilde{P})}\right]$$

in a Dyson series in powers of $\widetilde{P}$. If $m\geq 1$, the m^{th} term is

$$\begin{aligned}X_m:=\beta^m\int_0^1 ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{m-1}}ds_m\operatorname{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\\ \times\left[\mathrm{e}^{-\beta\widetilde{H}(1-s_1)}\widetilde{P}\mathrm{e}^{-\beta\widetilde{H}(s_1-s_2)}\widetilde{P}\cdots\widetilde{P}\mathrm{e}^{-\beta\widetilde{H}(s_{m-1}-s_m)}\widetilde{P}\mathrm{e}^{-\beta\widetilde{H}s_m}U_q\right].\end{aligned}$$

Recall that $\widetilde{P}:=\mathcal{P}^{\mathsf{hc}}_n P^{(q)}_V\mathcal{P}^{\mathsf{hc}}_n$ where

$$P^{(q)}_V=P_V\otimes I\otimes\cdots\otimes I+I\otimes P_V\otimes I\otimes\cdots\otimes I+\cdots+I\otimes\cdots\otimes I\otimes P_V \tag{3.15}$$

has q terms, so in the above trace we have m instances of this form. Let $P^{(q)}_r=I\otimes\cdots\otimes\underbrace{P_V}_{r^{th}\text{ place}}\otimes\cdots\otimes I$, and let $\widetilde{P}_r=\mathcal{P}^{\mathsf{hc}}_n P^{(q)}_r\mathcal{P}^{\mathsf{hc}}_n$.

Then we can write

$$\begin{aligned}X_m=\beta^m\int_0^1 ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{m-1}}ds_m\sum_{r_1=1}^{q}\cdots\sum_{r_m=1}^{q}\\ \times\operatorname{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\left[\mathrm{e}^{-\beta\widetilde{H}(1-s_1)}\widetilde{P}_{r_1}\mathrm{e}^{-\beta\widetilde{H}(s_1-s_2)}\widetilde{P}_{r_2}\cdots\widetilde{P}_{r_{m-1}}\mathrm{e}^{-\beta\widetilde{H}(s_{m-1}-s_m)}\widetilde{P}_{r_m}\mathrm{e}^{-\beta\widetilde{H}s_m}U_q\right].\end{aligned}$$

In terms of the basis of $\mathcal{H}^{\mathsf{hc}}_{q,n,V}$ we may write the expression for X_m as

$$X_m=\beta^m\int_0^1 ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{m-1}}ds_m\sum_{r_1=1}^{q}\cdots\sum_{r_m=1}^{q}\sum_{\mathbf{k}^0,\dots,\mathbf{k}^m}\sum_{\mathbf{i}^0\sim\mathbf{k}^0}\cdots\sum_{\mathbf{i}^m\sim\mathbf{k}^m}$$

$$\times \langle \mathbf{i}^0; \mathbf{k}^0 | e^{-\beta \widetilde{H}(1-s_1)} \widetilde{P}_{r_1} | \mathbf{i}^1; \mathbf{k}^1 \rangle \langle \mathbf{i}^1; \mathbf{k}^1 | e^{-\beta \widetilde{H}(s_1-s_2)} \widetilde{P}_{r_2} | \mathbf{i}^2; \mathbf{k}^2 \rangle \cdots$$
$$\times \cdots \langle \mathbf{i}^{m-1}; \mathbf{k}^{m-1} | e^{-\beta \widetilde{H}(s_{m-1}-s_m)} \widetilde{P}_{r_m} | \mathbf{i}^m; \mathbf{k}^m \rangle \langle \mathbf{i}^m; \mathbf{k}^m | e^{-\beta \widetilde{H} s_m} U_q | \mathbf{i}^0; \mathbf{k}^0 \rangle \quad (3.16)$$

where it is understood that the $\mathbf{i}$ summations are over $\Lambda_V^{(q)}$ and the $\mathbf{k}$ summations are over $\Lambda_{V+}^{(n-q)}$. Note that for $\mathbf{i} \sim \mathbf{k}$

$$\widetilde{P}_r |\mathbf{i}; \mathbf{k}\rangle = \frac{1}{V} \sum_{\substack{l=1\ldots V \\ l \notin \mathbf{k};\ l \neq i_1 \ldots \widehat{i_r} \ldots i_q}} |(i_1, \ldots, \widehat{i_r}, l, \ldots, i_q); \mathbf{k}\rangle \quad (3.17)$$

where again the hat symbol implies that the term is removed from the sequence.

Consider one of the inner products in the expression (3.16) for X_m, using (3.11) and (3.17) above. For $\mathbf{i} \sim \mathbf{k}$ and $\mathbf{j} \sim \mathbf{k}'$:

$$\begin{aligned}\langle \mathbf{i}; \mathbf{k} \,|\, e^{-\beta s \widetilde{H}} \widetilde{P}_r |\mathbf{j}; \mathbf{k}'\rangle &= \frac{e^{-\beta q s}}{V} \sum_{\substack{l=1\ldots V \\ l \notin \mathbf{k}';\, l \neq j_1, \ldots \widehat{j_r}, \ldots j_q}} \langle \mathbf{i} \,|\, (j_1, \ldots, \widehat{j_r}, l, \ldots, j_q)\rangle \langle \mathbf{k} \,|\, e^{-\beta s H^{\mathbf{i}}} |\mathbf{k}'\rangle \\ &= \frac{e^{-\beta q s}}{V} \sum_{\substack{l=1\ldots V \\ l \notin \mathbf{k}';\, l \neq j_1, \ldots, \widehat{j_r}, \ldots, j_q}} \delta_{i_1 j_1} \ldots \widehat{\delta_{i_r j_r}}\, \delta_{i_r l} \ldots \delta_{i_q j_q} \langle \mathbf{k} | e^{-\beta s H^{\mathbf{i}}} |\mathbf{k}'\rangle.\end{aligned}$$

In summing over l we replace l by i_r and the result is non-zero only if $i_r \notin \mathbf{k}'$ and $i_r \neq j_1, \ldots, \widehat{j_r}, \ldots, j_q$. However this last condition is not necessary because if $i_r = j_s$ $(s \neq r)$ then $j_s \neq i_s$ and we get zero. Also if for some $s \neq r$, $i_s \in \mathbf{k}'$ then once again $j_s \neq i_s$. We can therefore replace the condition $i_r \notin \mathbf{k}'$ by $\mathbf{i} \sim \mathbf{k}'$. Using $\mathcal{I}$ for the indicator function, we have

$$\begin{aligned}\langle \mathbf{i}; \mathbf{k} \,|\, e^{-\beta s \widetilde{H}} \widetilde{P}_r |\mathbf{j}; \mathbf{k}'\rangle &= \frac{e^{-\beta q s}}{V} \delta_{i_1 j_1} \ldots \widehat{\delta_{i_r j_r}} \ldots \delta_{i_q j_q} \langle \mathbf{k} | e^{-\beta s H^{\mathbf{i}}} |\mathbf{k}'\rangle \mathcal{I}_{(\mathbf{i} \sim \mathbf{k}')} \\ &= \frac{e^{-\beta q s}}{V} \delta_{i_1 j_1} \ldots \widehat{\delta_{i_r j_r}} \ldots \delta_{i_q j_q} \langle \mathbf{k} | \mathcal{P}_{\mathbf{i}}^{(n-q)} e^{-\beta s H^{\mathbf{i}}} \mathcal{P}_{\mathbf{i}}^{(n-q)} |\mathbf{k}'\rangle.\end{aligned}$$

Now if we sum over $\mathbf{j} \sim \mathbf{k}'$, with $\mathbf{i} \sim \mathbf{k}$ and for a fixed r:

$$\begin{aligned}\sum_{\mathbf{j} \sim \mathbf{k}'} \langle \mathbf{i}; \mathbf{k} | e^{-\beta \widetilde{H} s} \widetilde{P}_r |\mathbf{j}; \mathbf{k}'\rangle \langle \mathbf{j}; \mathbf{k}'| &= \frac{e^{-\beta s q}}{V} \langle \mathbf{k} | \mathcal{P}_{\mathbf{i}}^{(n-q)} e^{-\beta H^{\mathbf{i}} s} \mathcal{P}_{\mathbf{i}}^{(n-q)} |\mathbf{k}'\rangle \\ &\quad \times \sum_{\substack{j_r=1\ldots V \\ j_r \notin \mathbf{k}' \cup \mathbf{i} \setminus \{i_r\}}} \langle (i_1, \ldots, i_{r-1}, j_r, i_{r+1}, \ldots, i_q); \mathbf{k}'|.\end{aligned}$$

It is convenient to define the operation $[r, x](\mathbf{i})$ which inserts the value of x in the r^{th} position of $\mathbf{i}$ instead of i_r. So for example taking the ordered triplet $\mathbf{i} = (5, 4, 1)$, then $[2, 8](\mathbf{i}) = (5, 8, 1)$. For brevity we shall denote the composition of these operators as $[r_k, x_k; \ldots; r_2, x_2; r_1, x_1] := [r_k, x_k] \circ \cdots \circ [r_2, x_2] \circ [r_1, x_1]$.

Thus the final term in the above expression may be rewritten as $\langle [r, j_r](\mathbf{i}); \mathbf{k}'|$.

Performing two summations for fixed r_1 and r_2 we get:

$$\sum_{\mathbf{i}^1\sim\mathbf{k}^1}\sum_{\mathbf{i}^2\sim\mathbf{k}^2}\langle\mathbf{i}^0;\mathbf{k}^0|\mathrm{e}^{-\beta s\widetilde{H}}\widetilde{P}_{r_1}|\mathbf{i}^1;\mathbf{k}^1\rangle\langle\mathbf{i}^1;\mathbf{k}^1|\mathrm{e}^{-\beta t\widetilde{H}}\widetilde{P}_{r_2}|\mathbf{i}^2;\mathbf{k}^2\rangle\langle\mathbf{i}^2;\mathbf{k}^2|$$

$$=\frac{\mathrm{e}^{-\beta q(s+t)}}{V^2}\sum_{i^1_{r_1}\notin\mathbf{k}^1\cup\mathbf{i}^0\setminus\{i^0_{r_1}\}}\sum_{i^2_{r_2}\notin\mathbf{k}^2\cup[r_1,i^1_{r_1}](\mathbf{i}^0)\setminus\{i^0_{r_2}\}}\langle\mathbf{k}^0|\mathcal{P}_{\mathbf{i}^0}\,\mathrm{e}^{-\beta sH^{\mathbf{i}^0}}\,\mathcal{P}_{\mathbf{i}^0}|\mathbf{k}^1\rangle$$

$$\times\langle\mathbf{k}^1|\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\,\mathrm{e}^{-\beta tH^{[r_1,i^1_{r_1}](\mathbf{i}^0)}}\,\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}|\mathbf{k}^2\rangle\langle[r_1,i^1_{r_1};r_2,i^2_{r_2}](\mathbf{i}^0);\mathbf{k}^2|$$

$$=\frac{\mathrm{e}^{-\beta q(s+t)}}{V^2}\sum_{i^1_{r_1}\notin\mathbf{i}^0\setminus\{i^0_{r_1}\}}\sum_{i^2_{r_2}\notin\mathbf{k}^2\cup[r_1,i^1_{r_1}](\mathbf{i}^0)\setminus\{i^0_{r_2}\}}\langle\mathbf{k}^0|\,\mathcal{P}_{\mathbf{i}^0}\,\mathrm{e}^{-\beta sH^{\mathbf{i}^0}}\,\mathcal{P}_{\mathbf{i}^0}\,|\mathbf{k}^1\rangle$$

$$\times\langle\mathbf{k}^1|\,\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\,\mathrm{e}^{-\beta tH^{[r_1,i^1_{r_1}](\mathbf{i}^0)}}\,\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\,|\mathbf{k}^2\rangle\langle[r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0);\mathbf{k}^2|$$

due to the fact that $\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}|\mathbf{k}^1\rangle=0$ if $i^1_{r_1}\in\mathbf{k}^1$. We may apply this to all inner product terms of (3.16) except the final one. Note we sum over the V sites of the lattice, with certain points excluded in each case.

For the final inner product of (3.16) we obtain:

$$\langle[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0);\mathbf{k}^m|\mathrm{e}^{-\beta s_m\widetilde{H}}U_q|\mathbf{i}^0;\mathbf{k}^0\rangle$$

$$=\mathrm{e}^{-\beta qs_m}\langle[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0);\mathbf{k}^m|\mathrm{e}^{-\beta s_mH^{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}U_q|\mathbf{i}^0;\mathbf{k}^0\rangle$$

$$=\mathrm{e}^{-\beta qs_m}\langle\mathbf{k}^m|\mathrm{e}^{-\beta s_mH^{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}|\mathbf{k}^0\rangle\,\langle[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle$$

$$=\mathrm{e}^{-\beta qs_m}\langle\mathbf{k}^m|\mathcal{P}_{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta s_mH^{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}|\mathbf{k}^0\rangle$$

$$\times\langle[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle.$$

Applying this to the whole tracial expression of (3.16) we obtain

$$X_m=\mathrm{e}^{-\beta q}\frac{\beta^m}{V^m}\sum_{\mathbf{k}^0\ldots\mathbf{k}^m}\sum_{\mathbf{i}^0}\sum_{i^1_{r_1}\notin\mathbf{i}^0\setminus\{i^0_{r_1}\}}\sum_{i^2_{r_2}\notin[r_1,i^1_{r_1}](\mathbf{i}^0)\setminus\{i^1_{r_2}\}}\cdots\sum_{i^m_{r_m}\notin[r_{m-1},i^{m-1}_{r_{m-1}};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)\setminus\{i^{m-1}_{r_m}\}}$$

$$\times\langle\mathbf{k}^0|\mathcal{P}_{\mathbf{i}^0}\mathrm{e}^{-\beta(1-s_1)\widetilde{H}^{\mathbf{i}^0}}\mathcal{P}_{\mathbf{i}^0}|\mathbf{k}^1\rangle$$

$$\times\langle\mathbf{k}^1|\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta(s_1-s_2)\widetilde{H}^{[r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}|\mathbf{k}^2\rangle$$

$$\times\langle\mathbf{k}^2|\mathcal{P}_{[r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta(s_2-s_3)\widetilde{H}^{[r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}|\mathbf{k}^3\rangle$$

$$\ldots$$

$$\times\langle\mathbf{k}^m|\mathcal{P}_{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta s_m\widetilde{H}^{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}|\mathbf{k}^0\rangle$$

$$\times\langle[r_m,i^m_{r_m};\ldots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle$$

$$= \mathrm{e}^{-\beta q}\frac{\beta^m}{V^m}\sum_{\mathbf{i}^0}\sum_{i^1_{r_1}\notin\mathbf{i}^0\backslash\{i^0_{r_1}\}}\sum_{i^2_{r_2}\notin[r_1,i^1_{r_1}](\mathbf{i}^0)\backslash\{i^1_{r_2}\}}\cdots\sum_{i^m_{r_m}\notin[r_{m-1},i^{m-1}_{r_{m-1}};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)\backslash\{i^{m-1}_{r_m}\}}$$
$$\times\langle[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle$$
$$\times\,\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}}\Big[\mathcal{P}_{\mathbf{i}^0}\mathrm{e}^{-\beta(1-s_1)\widetilde{H}^{\mathbf{i}^0}}\mathcal{P}_{\mathbf{i}^0}\mathcal{P}_{i^1_{r_1}(\mathbf{i}^0)}\mathrm{e}^{-\beta(s_1-s_2)\widetilde{H}^{i^1_{r_1}(\mathbf{i}^0)}}\mathcal{P}_{i^1_{r_1}(\mathbf{i}^0)}\cdots$$
$$\times\cdots\mathcal{P}_{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta s_m\widetilde{H}^{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\Big].$$

From the Hölder inequality (see Manjegani [10]), for finite dimensional non-negative matrices $A_1, A_2, \dots, A_{m+1}$ we have the inequality

$$\big|\mathrm{trace}(A_1A_2\dots A_{m+1})\big|\le\mathrm{trace}\big|A_1A_2\dots A_{m+1}\big|\le\prod_{k=1}^{m+1}\big(\mathrm{trace}A_k^{p_k}\big)^{\frac{1}{p_k}}$$

where $\sum_{k=1}^{m+1}\frac{1}{p_k}=1$, $p_i>0$.

Set $p_1=\frac{1}{1-s_1}$, $p_2=\frac{1}{s_1-s_2}$, $\dots$, $p_m=\frac{1}{s_{m-1}-s_m}$, $p_{m+1}=\frac{1}{s_m}$. Taking the modulus of the above trace

$$\Big|\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}}\Big[\mathcal{P}_{\mathbf{i}^0}\mathrm{e}^{-\beta\widetilde{H}^{\mathbf{i}^0}(1-s_1)}\mathcal{P}_{\mathbf{i}^0}\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta\widetilde{H}^{[r_1,i^1_{r_1}](\mathbf{i}^0)}(s_1-s_2)}\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\cdots$$
$$\times\cdots\mathcal{P}_{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta\widetilde{H}^{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}(s_m)}\mathcal{P}_{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\Big]\Big|$$
$$\le\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}}\Big[\mathcal{P}_{\mathbf{i}^0}\mathrm{e}^{-\beta\widetilde{H}^{\mathbf{i}^0}}\mathcal{P}_{\mathbf{i}^0}\Big]^{1-s_1}\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{n-q,V}}\Big[\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta\widetilde{H}^{[r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_1,i^1_{r_1}](\mathbf{i}^0)}\Big]^{s_1-s_2}\cdots$$
$$\times\cdots\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}}\Big[\mathcal{P}_{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\mathrm{e}^{-\beta\widetilde{H}^{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}}\mathcal{P}_{[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)}\Big]^{s_m}.$$

Since the trace is independent of the $V-q$ sites $\{\mathbf{i}^0,[r_1,i^1_{r_1}](\mathbf{i}^0),\dots,[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)\}$, and therefore using Remark 3.3, the product of all the trace terms above is equal to

$$\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}}\big[\mathcal{P}_{\mathbf{l}}\mathrm{e}^{-\beta\widetilde{H}^{\mathbf{l}}}\mathcal{P}_{\mathbf{l}}\big]$$

with $\mathbf{l}=\{V-q+1,V-q+2,\dots,V\}$ and from Remark 3.2,

$$\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{(n-q),V,+}}\big[\mathcal{P}_{\mathbf{l}}\mathrm{e}^{-\beta\widetilde{H}^{\mathbf{l}}}\mathcal{P}_{\mathbf{l}}\big]=Z_\beta((V-q)/V,n-q,V-q).\tag{3.18}$$

Consider the sum

$$\sum_{\mathbf{i}^0}\sum_{i^1_{r_1}\notin\mathbf{i}^0\backslash\{i^0_{r_1}\}}\sum_{i^2_{r_2}\notin[r_1,i^1_{r_1}](\mathbf{i}^0)\backslash\{i^1_{r_2}\}}\cdots$$
$$\times\cdots\sum_{i^m_{r_m}\notin[r_{m-1},i^{m-1}_{r_{m-1}};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)\backslash\{i^{m-1}_{r_m}\}}\langle[r_m,i^m_{r_m};\dots;r_2,i^2_{r_2};r_1,i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle.\tag{3.19}$$

If $\{r_1, r_2, \ldots, r_m\} \neq \{1, 2, \ldots, q\}$, then $|[r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0)\rangle$ is of the form

$$|j_1, j_2, \ldots, j_{n_1}, i^0_{n_1+1}, \ldots, i^0_{n_2}, j_{n_2+1}, \ldots, j_{n_3}, i^0_{n_3+1}, \ldots, i^0_{n_4}, j_{n_4+1}, \ldots\ldots\rangle$$

where $\{n_1, n_2, \ldots\}$ is a non-empty ordered set of distinct integers between 0 and q. This state is clearly orthogonal to $U_q\mathbf{i}^0$ for any q. Note that this situation does not arise if $q = 1$. Note also that this is always the case if $m < q$.

We may bound the remaining sum corresponding to terms for which $\{r_1, r_2, \ldots, r_m\} = \{1, 2, \ldots, q\}$ by

$$\leq \sum_{\mathbf{i}^0} \underbrace{\sum_{i^1_{r_1}=1}^{V} \sum_{i^2_{r_2}=1}^{V} \cdots \sum_{i^m_{r_m}=1}^{V}}_{\substack{\text{where } [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}] \\ \text{has distinct indices}}} \langle [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle.$$

Observe that in this case $|[r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0)\rangle$ is independent of $\mathbf{i}^0$ so we may take it to be

$$|[r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{s}^0)\rangle$$

where $\mathbf{s}^0 = (1, 2, 3, \ldots, q)$. Then we can interchange the $\mathbf{i}^0$ summation with the others, and for each choice of $i^1_{r_1}, i^2_{r_2}, \ldots, i^m_{r_m}$ there exists only one possible $\mathbf{i}^0 \in \Lambda^{(q)}_V$ such that

$$\langle [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle \neq 0.$$

So we may conclude that

$$\begin{aligned}
&\sum_{\mathbf{i}^0} \sum_{i^1_{r_1} \notin \mathbf{i}^0 \setminus \{i^0_{r_1}\}} \sum_{i^2_{r_2} \notin [r_1, i^1_{r_1}](\mathbf{i}^0) \setminus \{i^1_{r_2}\}} \cdots \\
&\quad \times \cdots \sum_{i^m_{r_m} \notin [r_{m-1}, i^{m-1}_{r_{m-1}}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0) \setminus \{i^{m-1}_{r_m}\}} \langle [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle \leq V^m.
\end{aligned} \tag{3.20}$$

Applying this, we see that the modulus of the integrated m^{th} term of the Dyson series may bounded above by

$$\begin{aligned}
|X_m| &\leq \mathrm{e}^{-\beta q} \frac{\beta^m}{m!} \frac{1}{V^m} Z_\beta((V-q)/V, n-q, V-q) \sum_{r_1=1}^{q} \cdots \sum_{r_m=1}^{q} \\
&\quad \times \sum_{\mathbf{i}^0} \sum_{i^1_{r_1} \notin \mathbf{i}^0 \setminus \{i^0_{r_1}\}} \sum_{i^2_{r_2} \notin [r_1, i^1_{r_1}](\mathbf{i}^0) \setminus \{i^1_{r_2}\}} \cdots \\
&\quad \times \cdots \sum_{i^m_{r_m} \notin [r_{m-1}, i^{m-1}_{r_{m-1}}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0) \setminus \{i^{m-1}_{r_m}\}} \langle [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0)|U_q\mathbf{i}^0\rangle \\
&\leq \mathrm{e}^{-\beta q} \frac{\beta^m}{m!} \frac{1}{V^m} Z_\beta((V-q)/V, n-q, V-q) \sum_{r_1=1}^{q} \cdots \sum_{r_m=1}^{q} V^m \\
&= \mathrm{e}^{-\beta q} \frac{q^m \beta^m}{m!} Z_\beta((V-q)/V, n-q, V-q).
\end{aligned}$$

Noting that the zeroth term of the Dyson series is

$$X_0 = \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}\big[U_q \mathrm{e}^{-\beta \widetilde{H}}\big],$$

we may re-sum the series to obtain

$$\begin{aligned}&\Big|\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}\big[U_q \mathrm{e}^{-\beta H^{\mathrm{hc}}_{n,V}}\big] - \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}\big[U_q \mathrm{e}^{-\beta \widetilde{H}}\big]\Big|\\ &\quad\le \mathrm{e}^{-\beta q} Z_\beta((V-q)/V, n-q, V-q) \sum_{m=1}^{\infty} \frac{q^m \beta^m}{m!}.\end{aligned}$$

Thus

$$\begin{aligned}|c^n_V(q) - \widetilde{c}^n_V(q)| &= \frac{1}{V}\left|\frac{\mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}[U_q \mathrm{e}^{-\beta H^{\mathrm{hc}}_{n,V}}] - \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{q,n,V}}[U_q \mathrm{e}^{-\beta \widetilde{H}}]}{Z_\beta(n,V)}\right|\\ &\le \frac{\mathrm{e}^{-\beta q}}{V}\,\frac{Z_\beta((V-q)/V, n-q, V-q)}{Z_\beta(n,V)} \sum_{m=1}^{\infty}\frac{q^m\beta^m}{m!}\\ &= \frac{\mathrm{e}^{-\beta q}}{V}(\mathrm{e}^{\beta q}-1)\frac{Z_\beta((V-q)/V, n-q, V-q)}{Z_\beta(n,V)}.\end{aligned}$$

3.3 Proof of Proposition 3.3

Recall that we have

$$\begin{aligned}Z_\beta(n-q, V-q) &= \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{n-q,V-q,+}}[\mathrm{e}^{-\beta H^{\mathrm{hc}}_{n-q,V-q}}]\\ &= \mathrm{e}^{-\beta(n-q)}\ \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{n-q,V-q,+}}\big[\mathrm{e}^{\beta \mathcal{P}^{\mathrm{hc}}_{n-q} P^{n-q}_{V-q} \mathcal{P}^{\mathrm{hc}}_{n-q}}\big]\end{aligned} \tag{3.21}$$

while

$$\begin{aligned}Z_\beta((V-q)/V, n-q, V-q) &= \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{n-q,V-q,+}}[\mathrm{e}^{-\beta H^{\mathrm{hc}}_{(V-q)/V,n-q,V-q}}]\\ &= \mathrm{e}^{-\beta(n-q)}\ \mathrm{trace}_{\mathcal{H}^{\mathrm{hc}}_{n-q,V-q,+}}\big[\mathrm{e}^{\beta(\frac{V-q}{V})\mathcal{P}^{\mathrm{hc}}_{n-q} P^{n-q}_{V-q} \mathcal{P}^{\mathrm{hc}}_{n-q}}\big].\end{aligned} \tag{3.22}$$

Comparison of (3.21) and (3.22) yields

$$Z_\beta((V-q)/V, n-q, V-q) = \mathrm{e}^{-\beta\frac{q}{V}(n-q)}\ Z_{\beta(\frac{V-q}{V})}(n-q, V-q)$$

and thus we have to analyse the following ratio:

$$\frac{\mathrm{e}^{-\beta\frac{q}{V}(n-q)} Z_{\beta(\frac{V-q}{V})}(n-q, V-q)}{Z_\beta(n,V)}. \tag{3.23}$$

Penrose in [13] gave an explicit expression for $Z_\beta(n,V)$:

$$Z_\beta(n,V) = \sum_{r=0}^{\min(n,V-n)} z(r,n,V,\beta),$$

where

$$z(r,n,V,\beta):=\left(\frac{V-2r+1}{V-r+1}\right)\binom{V}{r}\exp\left\{-\frac{\beta}{V}\left[Vr-r^2+r+n^2-n\right]\right\}.$$

He also proved that if $h_V:[0,\min(\rho,1-\rho)]\to\mathbb{R}$ converges uniformly in $[0,\min(\rho,1-\rho)]$ as $V\to\infty$ to a continuous function $h:[0,\min(\rho,1-\rho)]\to\mathbb{R}$, then

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}}\frac{1}{Z_\beta(n,V)}\sum_{r=0}^{\min(n,V-n)}h_V\left(\frac{r}{V}\right)z(r,n,V,\beta)=\begin{cases}h(\rho), & \text{if } \rho\in[0,\rho_\beta],\\ h(\rho_\beta), & \text{if } \rho\in[\rho_\beta,1-\rho_\beta],\\ h(1-\rho), & \text{if } \rho\in[1-\rho_\beta,1].\end{cases} \tag{3.24}$$

We wish to express the ratio in (3.23) in the form of the lefthand side of (3.24). We have

$$Z_{\beta(\frac{V-q}{V})}(n-q,V-q)=\sum_{r=0}^{\min(n-q,V-n)}\left(\frac{V-q-2r+1}{V-q-r+1}\right)\binom{V-q}{r}$$
$$\times\exp\left\{-\frac{\beta}{V}\left[r(V-q)-r^2+r+(n-q)^2-(n-q)\right]\right\}.$$

For the case $\rho>\frac{1}{2}$, for large V, $n-q>V-n$ we must sum from zero to $V-n$ and a straightforward calculation then gives

$$\mathrm{e}^{-\beta\frac{q}{V}(n-q)}Z_{\beta(\frac{V-q}{V})}(n-q,V-q)=\sum_{r=0}^{V-n}h_V\left(\frac{r}{V}\right)z(r,n,V,\beta)$$

where

$$h_V(x)=\left(\frac{1-2x-(q-1)/V}{1-2x+1/V}\right)\left(\frac{1-x+1/V}{1-x-(q-1)/V}\right)$$
$$\times\prod_{s=0}^{q-1}\left(\frac{1-x-s/V}{1-s/V}\right)\exp\left\{\beta q\left[x+\rho-1/V\right]\right\}. \tag{3.25}$$

Therefore

$$h(x)=\lim_{V\to\infty}h_V(x)=(1-x)^q\,\mathrm{e}^{q\beta(x+\rho)}. \tag{3.26}$$

It is clear that the convergence is uniform since $h_V(x)$ is a product of terms each of which converges uniformly on $[0,1-\rho]$ for $\rho>\frac{1}{2}$. Thus

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}}\frac{\mathrm{e}^{-\beta\frac{q}{V}(n-q)}Z_{\beta(\frac{V-q}{V})}(n-q,V-q)}{Z_\beta(n,V)}=\begin{cases}(1-\rho_\beta)^q\,\mathrm{e}^{q\beta(\rho_\beta+\rho)} & \text{if } \rho\in(1/2,1-\rho_\beta],\\ \rho^q\mathrm{e}^{\beta q} & \text{if } \rho\in(1-\rho_\beta,1].\end{cases}$$

Note that using the relation

$$\beta=\frac{1}{1-2\rho_\beta}\ln\left(\frac{1-\rho_\beta}{\rho_\beta}\right)$$

we get

$$(1-\rho_\beta)^q\, e^{q\beta(\rho_\beta+\rho)} = \rho_\beta^q\, e^{q\beta(1+\rho-\rho_\beta)}$$

and therefore we have proved Proposition 3.3 for $\rho > \frac{1}{2}$. For the case $\rho \le \frac{1}{2}$ we have that $n-q < V-n$, the sum for $e^{-\beta\frac{q}{V}(n-q)} Z_{\beta(\frac{V-q}{V})}(n-q, V-q)$ is up to $n-q$, and therefore we need to shift the index by q to get it into the required form. After shifting we get

$$\begin{aligned} e^{-\beta\frac{q}{V}(n-q)} Z_{\beta(\frac{V-q}{V})}(n-q, V-q) = \sum_{r=q}^{n} z(r,n,V,\beta) &\left(\frac{V+q-2r+1}{V-2r+1}\right) \\ &\times \frac{r(r-1)(r-2)\cdots(r-q+1)}{V(V-1)(V-2)\cdots(V-q+1)} \\ &\times \exp\left\{\frac{\beta q}{V}\left[V+n-r\right]\right\}. \end{aligned}$$

Note that summand is zero if we put $r = 0, \ldots, q-1$. Thus we may sum from zero to n to get as before

$$e^{-\beta\frac{q}{V}(n-q)} Z_{\beta(\frac{V-q}{V})}(n-q, V-q) = \sum_{r=0}^{n} h_V\left(\frac{r}{V}\right) z(r,n,V,\beta)$$

where this time

$$h_V(x) = \left(\frac{1-2x+(q+1)/V}{1-2x+1/V}\right) \prod_{s=0}^{q-1} \left(\frac{x-s/V}{1-s/V}\right) \exp\left\{\beta q\left[1+\rho-x\right]\right\} \tag{3.27}$$

so that

$$h(x) = \lim_{\substack{n,V\to\infty \\ n/V=\rho}} h_V(x) = x^q \exp\{\beta q(1+\rho-x)\}.$$

Convergence is again uniform on $[0,\rho]$ for $\rho < \frac{1}{2}$ and therefore

$$\lim_{\substack{n,V\to\infty \\ n/V=\rho}} \frac{e^{-\beta\frac{q}{V}(n-q)} Z_{\beta(\frac{V-q}{V})}(n-q, V-q)}{Z_\beta(n,V)} = \begin{cases} \rho^q e^{\beta q} & \text{if } \rho \in [0,\rho_\beta), \\ \rho_\beta^q\, e^{q\beta(1+\rho-\rho_\beta)} & \text{if } \rho \in [\rho_\beta, 1/2), \end{cases}$$

proving Proposition 3.3 for $\rho < \frac{1}{2}$. The case $\rho = \frac{1}{2}$ is more delicate because the first term in (3.27) does not converge uniformly. We can write (taking $V = 2n$)

$$h_{2n}(r/2n) = \widetilde{h}_{2n}(r/2n) + \frac{q}{2(n-r)+1}\widetilde{h}_{2n}(r/2n)$$

where

$$\widetilde{h}_{2n}(x) = \prod_{s=0}^{q-1}\left(\frac{x-s/2n}{1-s/2n}\right) \exp\left\{\beta q\left[3/2-x\right]\right\}.$$

Clearly $\widetilde{h}_{2n}(x)$ converges uniformly on $[0, 1/2]$ and therefore

$$\lim_{n\to\infty} \frac{1}{Z_\beta(n,2n)} \sum_{r=0}^{n} \widetilde{h}_{2n}\left(\frac{r}{2n}\right) z(r,n,2n,\beta) = \rho_\beta^q\, e^{\beta q(3/2-\rho_\beta)}.$$

We thus have to show that

$$\lim_{n\to\infty}\frac{1}{Z_\beta(n,2n)}\sum_{r=0}^{n}\frac{\widetilde{h}_{2n}(\frac{r}{2n})}{2(n-r)+1}\,z(r,n,2n,\beta)=0.$$

Since $\widetilde{h}_{2n}(x)$ is bounded, by C say,

$$\lim_{n\to\infty}\frac{1}{Z_\beta(n,2n)}\sum_{r<n-n^{1/4}}\frac{\widetilde{h}_{2n}(\frac{r}{2n})}{2(n-r)+1}\,z(r,n,2n,\beta)\le\lim_{n\to\infty}\frac{C}{2n^{1/4}}=0.$$

On the other hand one can prove that for $n-2n^{1/2}\le r\le n-n^{1/2}$ and $r'\ge n-n^{1/4}$

$$\ln z(r,n,2n,\beta)-\ln z(r',n,2n,\beta)>\frac{1}{8}\ln n$$

for n large, so that $z(r',n,2n,\beta)/z(r,n,2n,\beta)<1$. Therefore

$$\begin{aligned}
&\lim_{n\to\infty}\frac{1}{Z_\beta(n,2n)}\sum_{r\ge n-n^{1/4}}\frac{\widetilde{h}_{2n}(\frac{r}{2n})}{2(n-r)+1}z(r,n,2n,\beta)\\
&\quad\le\lim_{n\to\infty}C\frac{\sum_{r\ge n-n^{1/4}}z(r,n,2n,\beta)}{\sum_{n-2n^{1/2}\le r\le n-n^{1/2}}z(r,n,2n,\beta)}\\
&\quad\le\lim_{n\to\infty}\frac{C}{n^{1/4}}\frac{\max_{r\ge n-n^{1/4}}z(r,n,2n,\beta)}{\min_{n-2n^{1/2}\le r\le n-n^{1/2}}z(r,n,2n,\beta)}\le\lim_{n\to\infty}\frac{C}{n^{1/4}}=0.
\end{aligned}$$

3.4 Proof of Proposition 3.4

Recall that

$$\widetilde{c}_V^{\,n}(q)=\frac{1}{Z_\beta(n,V)}\frac{1}{V}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\left[U_q\mathrm{e}^{-\beta\widetilde{H}^{\mathsf{hc}}_{q,n,V}}\right].$$

Considering the trace over $\mathcal{H}^{\mathsf{hc}}_{q,n,V}$, expanding it in terms of its basis $\{|\mathbf{i};\mathbf{k}\rangle\}$ and using Remark 3.1 above, where $\mathbf{i}\sim\mathbf{k}$

$$\begin{aligned}
\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}}\left[U_q\mathrm{e}^{-\beta\widetilde{H}^{\mathsf{hc}}_{q,n,V}}\right]&=\sum_{\mathbf{k}}\sum_{\mathbf{i}\sim\mathbf{k}}\langle\mathbf{i};\mathbf{k}|U_q\mathrm{e}^{-\beta\mathcal{P}^{\mathsf{hc}}_n(n-P_V^{(n-q)})\mathcal{P}^{\mathsf{hc}}_n}|\mathbf{i};\mathbf{k}\rangle\\
&=\mathrm{e}^{-\beta q}\sum_{\mathbf{k}}\sum_{\mathbf{i}\sim\mathbf{k}}\langle U_q\mathbf{i};\mathbf{k}|\mathrm{e}^{-\beta H^{\mathbf{i}}}|\mathbf{i};\mathbf{k}\rangle\\
&=\mathrm{e}^{-\beta q}\sum_{\mathbf{k}}\sum_{\mathbf{i}\sim\mathbf{k}}\langle U_q\mathbf{i}|\mathbf{i}\rangle\langle\mathbf{k}|\mathrm{e}^{-\beta H^{\mathbf{i}}}|\mathbf{k}\rangle.
\end{aligned}$$

For $q>1$, an element of the basis of the unsymmetrised q-space $\mathcal{H}_V^{(q)}$ may be written as an ordered q-tuple $\mathbf{i}=(i_1,i_2,\dots,i_q)$ where the i_l's are all distinct. Then we may write

$$\begin{aligned}
\langle U_q\mathbf{i}|\mathbf{i}\rangle&=\langle U_q(\mathbf{e}_{i_1}\otimes\mathbf{e}_{i_2}\otimes\cdots\otimes\mathbf{e}_{i_q})\,|\,\mathbf{e}_{i_1}\otimes\mathbf{e}_{i_2}\otimes\cdots\otimes\mathbf{e}_{i_q}\rangle\\
&=\langle\mathbf{e}_{i_2}\otimes\mathbf{e}_{i_3}\otimes\cdots\otimes\mathbf{e}_{i_q}\otimes\mathbf{e}_{i_1}\,|\,\mathbf{e}_{i_1}\otimes\mathbf{e}_{i_2}\otimes\cdots\otimes\mathbf{e}_{i_q}\rangle=0.
\end{aligned}$$

Hence $\widetilde{c}_V^n(q)$ is non-zero only if $q = 1$.

For the second statement, note that we may re-express $\widetilde{c}_V^n(1)$ as follows:

$$\begin{aligned}\widetilde{c}_V^n(1) &= \frac{1}{Z_\beta(n,V)}\frac{1}{V}\operatorname{trace}_{\mathcal{P}_n^{\mathsf{hc}}(\mathcal{H}_V^{(1)}\otimes\mathcal{H}_{V,+}^{(n-1)})}\big[\mathrm{e}^{-\beta\widetilde{H}_{1,n,V}^{\mathsf{hc}}}\big]\\ &= \frac{\mathrm{e}^{-\beta}}{Z_\beta(n,V)}\frac{1}{V}\sum_{i=1}^{V}\sum_{\mathbf{k}/\ni i}\langle\mathbf{k}|\mathrm{e}^{-\beta H^i}|\mathbf{k}\rangle\\ &= \frac{\mathrm{e}^{-\beta}}{Z_\beta(n,V)}\frac{1}{V}\sum_{i=1}^{V}\operatorname{trace}_{\mathcal{H}_{n-1,V,+}^{\mathsf{hc}}}\big[\mathcal{P}_i\mathrm{e}^{-\beta H^i}\mathcal{P}_i\big]\\ &= \mathrm{e}^{-\beta}\,\frac{Z_\beta(\frac{V-1}{V},n-1,V-1)}{Z_\beta(n,V)}\end{aligned}$$

and the result follows from Proposition 3.3.

4 ODLRO

The one-body reduced density matrix for $x, x' \in \Lambda_V$ may be defined as

$$D_{\beta,n,V}(x,x') := \langle a_x^* a_{x'}\rangle = \frac{1}{Z_\beta(n,V)}\operatorname{trace}_{\mathcal{H}_{n,V,+}^{\mathsf{hc}}}\big[K_{x,x'}^{(n)}\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\big] \tag{4.1}$$

where for $\phi \in \mathcal{H}_V$, $K_{x,x'}\phi = \langle \mathbf{e}_{x'}|\phi\rangle\mathbf{e}_x$.

Penrose showed that for $x \neq x'$,

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}} D_{\beta,n,V}(x,x') = \rho_\beta^c,$$

that is, whenever Bose-Einstein condensation occurs, there is *Off-diagonal long-range order* as defined by Yang [21]. It has been argued and proved in some cases (see for example [19] and [5]) that in the expansion of $D_{\beta,n,V}(x,x')$ in terms of permutation cycles, only infinite cycles contribute to long-range order. Here we are able to show this explicitly.

By the proposition in the Appendix, we have

$$D_{\beta,n,V}(x,x') = \sum_{q=1}^{n} C_V^n(q;K_{x,x'})$$

where

$$C_V^n(q;K_{x,x'}) = \frac{1}{Z_\beta(n,V)}\operatorname{trace}_{\mathcal{H}_{q,n,V}^{\mathsf{hc}}}\big[(K_{x,x'}\otimes I\otimes I\otimes\cdots\otimes I)U_q\mathrm{e}^{-\beta H_{n,V}^{\mathsf{hc}}}\big]. \tag{4.2}$$

Note that this is equivalent to the expansion of $\sigma_\rho(x)$ in (2.14) and (2.16) in [19].

Applying the argument in Sects. 3.2 and 3.3, we can show that

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}} C_V^n(q;K_{x,x'}) = \lim_{\substack{n,V\to\infty\\ n/V=\rho}} \widetilde{C}_V^n(q;K_{x,x'}) \tag{4.3}$$

where we take

$$\widetilde{C}_V^n(q; K_{x,x'}) = \frac{1}{Z_\beta(n, V)} \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}} \left[(K_{x,x'} \otimes I \otimes I \otimes \cdots \otimes I) U_q \mathrm{e}^{-\beta \widetilde{H}^{\mathsf{hc}}_{q,n,V}}\right].$$

The only difference is that instead of (3.19), we obtain

$$\sum_{\mathbf{i}^0} \sum_{i^1_{r_1} \notin \mathbf{i}^0 \setminus \{i^0_{r_1}\}} \sum_{i^2_{r_2} \notin [r_1, i^1_{r_1}](\mathbf{i}^0) \setminus \{i^1_{r_2}\}} \cdots \sum_{i^m_{r_m} \notin [r_{m-1}, i^{m-1}_{r_{m-1}}; \ldots; r_1, i^1_{r_1}](\mathbf{i}^0) \setminus \{i^{m-1}_{r_m}\}} \\ \times \langle [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{i}^0) | (K_{x,x'} \otimes I \otimes \cdots \otimes I) U_q \mathbf{i}^0 \rangle \tag{4.4}$$

whose treatment is similar but slightly more complicated, as detailed below.

Let $q > 1$ and consider the case $\{r_1, r_2, \ldots, r_m\} \neq \{1, 2, \ldots, q\}$. When $1 \notin \{r_1, r_2, \ldots, r_m\}$ we obtain inner products of the form:

$$\langle i^0_1 | K_{x,x'} i^0_2 \rangle \langle j_2, j_3, \ldots, j_q | i^0_3, i^0_4, \ldots, i^0_q, i^0_1 \rangle$$

where $j_k \neq i^0_1$ for all k by the hard-core condition, implying the second term is zero as $j_q \neq i^0_1$. On the other hand, when $1 \in \{r_1, r_2, \ldots, r_m\}$, then there exists at least one $l \notin \{r_1, r_2, \ldots, r_m\}$, yielding an inner product of the form

$$\langle j_1 | K_{x,x'} i^0_2 \rangle \langle j_2, \ldots, j_{l-1}, i_l, j_{l+1}, \ldots, j_q | i^0_3, i^0_4, \ldots, i^0_q, i^0_1 \rangle$$

which also results in the second term being zero as $\langle i_l | i_{l+1} \rangle = 0$. Note that the above cases do not occur for $q = 1$.

For the case $\{r_1, r_2, \ldots, r_m\} = \{1, \ldots, q\}$, as before, the remaining sum may be bounded by a similar expression whose summations have slightly relaxed restrictions. Also the left hand side of the inner product is independent of $\mathbf{i}^0$, so again denoting $\mathbf{s}^0 = (1, 2, 3, \ldots, q)$, we have

$$\leq \underbrace{\sum_{i^1_{r_1}=1}^{V} \sum_{i^2_{r_2}=1}^{V} \cdots \sum_{i^m_{r_m}=1}^{V}}_{\substack{\text{where } [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{s}^0) \\ \text{has distinct indices}}} \sum_{\mathbf{i}^0} \langle [r_m, i^m_{r_m}; \ldots; r_2, i^2_{r_2}; r_1, i^1_{r_1}](\mathbf{s}^0) | (K_{x,x'} i^0_2), i^0_3, \ldots, i^0_q, i^0_1 \rangle \tag{4.4}$$

and as there is only one possible value for each $i^0_1, i^0_3, i^0_4, \ldots, i^0_q$ giving a non-zero summand, we can bound above by

$$\leq \sum_{i^1_{r_1}=1}^{V} \sum_{i^2_{r_2}=1}^{V} \cdots \sum_{i^m_{r_m}=1}^{V} \sum_{i^0_2=1}^{V} \langle i^k_{r_k} | K_{x,x'} i^0_2 \rangle = V^{m-1} \sum_{i^k_{r_k}=1}^{V} \sum_{i^0_2=1}^{V} \langle i^k_{r_k} | K_{x,x'} i^0_2 \rangle = V^{m-1}$$

where $k \in [1, m]$ is the smallest number such that $r_k = 1$, and for any $x, x' \in \Lambda_V$. Thus the entire sum (4.4) is bounded above by V^{m-1}. Therefore one can conclude the argument of Sect. 3.3, proving (4.3).

Moreover, following the reasoning in Sect. 3.4, we can then check that for $q \geq 1$ and $x \neq x'$, $\widetilde{C}_V^n(q; K_{x,x'}) = 0$, since for $q = 1$, $\langle \mathbf{e}_i | K_{x,x'} \mathbf{e}_i \rangle = 0$, and for $q > 1$

$$\langle (K_{x,x'} \otimes I \otimes \cdots \otimes I) U_q \mathbf{i} | \mathbf{i} \rangle = \langle (K_{x,x'} \mathbf{e}_{i_2}) \otimes \mathbf{e}_{i_3} \otimes \cdots \otimes \mathbf{e}_{i_q} \otimes \mathbf{e}_{i_1} \,|\, \mathbf{e}_{i_1} \otimes \mathbf{e}_{i_2} \otimes \cdots \otimes \mathbf{e}_{i_q} \rangle = 0$$

as the i_l's are all distinct. So we have that

$$\lim_{\substack{n,V\to\infty\\ n/V=\rho}} C_V^n(q; K_{x,x'}) = 0$$

and that

$$\lim_{Q\to\infty} \lim_{\substack{n,V\to\infty\\ n/V=\rho}} \sum_{q=Q+1}^{\infty} C_V^n(q; K_{x,x'}) = \lim_{\substack{n,V\to\infty\\ n/V=\rho}} D_{\beta,n,V}(x,x') = \rho_\beta^c.$$

Appendix: Expectation of Operator in Terms of Cycle Lengths

Proposition A.1 *Given an operator A on $\mathcal{H}_V$, the expectation of A may be expressed in terms of cycle lengths*

$$\langle A^{(n)}\rangle = \sum_{q=0}^{n} C_V^n(q; A) \tag{A.1}$$

where

$$C_V^n(q; A) = \frac{1}{Z_\beta(n,V)} \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{q,n,V}} \left[(A\otimes I\otimes\cdots\otimes I)U_q \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]. \tag{A.2}$$

Note that $c_V^n(q) = C_V^n(q; I)/V$ where $c_V^n(q)$ is as defined in Proposition 3.1.

Proof

$$\langle A^{(n)}\rangle = \frac{1}{Z_\beta(n,V)}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V,+}}\left[A^{(n)}\mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right] = \frac{1}{Z_\beta(n,V)}\frac{1}{n!}\sum_{\pi\in S_n}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[A^{(n)}U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]$$

using the facts that $[U_\pi, H^{\mathsf{hc}}_{n,V}]=0$, $[U_\pi, \mathcal{P}^{\mathsf{hc}}_n]=0$ and by the cyclicity of the trace. Note we can simplify this expression by the following method:

$$\begin{aligned}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[A^{(n)}U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right] &= \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[\sum_{i=1}^{n}(I\otimes\cdots\otimes \underbrace{A}_{i\text{th position}} \otimes\cdots\otimes I)U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]\\ &= \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[\sum_{i=1}^{n}U_{(1i)}(A\otimes I\otimes\cdots\otimes I)U_{(1i)}U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]\end{aligned}$$

where $U_{(1i)}$ represents the transposition $(1\,i)$, so using cyclicity of the trace again

$$\begin{aligned}&= \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[\sum_{i=1}^{n}(A\otimes I\otimes\cdots\otimes I)U_{(1i)}U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}U_{(1i)}\right]\\ &= \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[\sum_{i=1}^{n}(A\otimes I\otimes\cdots\otimes I)U_{(1i)}U_\pi U_{(1i)}\mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]\\ &= n\ \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\left[(A\otimes I\otimes\cdots\otimes I)U_{\pi'}\mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\right]\end{aligned}$$

where $\pi' = (1\,i)\,\pi\,(i\;1)$ using (3.10). Thus

$$\langle A^{(n)}\rangle = \frac{1}{Z_\beta(n,V)}\frac{1}{(n-1)!}\sum_{\pi\in S_n}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\Big[(A\otimes I\otimes\cdots\otimes I)U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\Big]. \tag{A.3}$$

Given distinct indices $i_2,\dots,i_q$, let

$$S_n^q(i_2,i_3,\dots i_q) = \Big\{\pi\in S_n : \pi(i_m)=i_{m+1},\ 1\le m<q \text{ with } i_1=\pi(i_q)=1\Big\}.$$

Then for any $\pi\in S_n^q(i_2,i_3,\dots i_q)$, there exists a $\pi'\in S_{n-q}$ so that one can write

$$\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\Big[(A\otimes I\otimes\cdots\otimes I)U_\pi \mathrm{e}^{-\beta H}\Big] = \mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\Big[(A\otimes I\otimes\cdots\otimes I)(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H}\Big].$$

The set $S_n^q(i_2,i_3,\dots i_q)$ form a partition of the set of permutations where 1 belongs to a cycle of length q. There are $\frac{(n-1)!}{(n-q)!}$ such sets. Then

$$\begin{aligned}
\langle A^{(n)}\rangle &= \frac{1}{Z_\beta(n,V)}\frac{1}{(n-1)!}\sum_{\pi\in S_n}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\Big[(A\otimes I\otimes\cdots\otimes I)U_\pi \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\Big]\\
&= \frac{1}{Z_\beta(n,V)}\frac{1}{(n-1)!}\sum_{q=1}^{n}\frac{(n-1)!}{(n-q)!}\\
&\quad\times\sum_{\pi'\in S_{n-q}}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\Big[(A\otimes I\otimes\cdots\otimes I)(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\Big]\\
&= \frac{1}{Z_\beta(n,V)}\sum_{q=1}^{n}\frac{1}{(n-q)!}\sum_{\pi'\in S_{n-q}}\mathrm{trace}_{\mathcal{H}^{\mathsf{hc}}_{n,V}}\Big[(A\otimes I\otimes\cdots\otimes I)(U_q\otimes U_{\pi'})\mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\Big]\\
&= \frac{1}{Z_\beta(n,V)}\sum_{q=1}^{n}\mathrm{trace}_{\mathcal{P}^{\mathsf{hc}}_n(\mathcal{H}_V^{(q)}\otimes\mathcal{H}_{V,+}^{(n-q)})}\Big[(A\otimes I\otimes\cdots\otimes I)U_q \mathrm{e}^{-\beta H^{\mathsf{hc}}_{n,V}}\Big]
\end{aligned}$$

and recall that $\mathcal{H}^{\mathsf{hc}}_{q,n,V} := \mathcal{P}^{\mathsf{hc}}_n(\mathcal{H}_V^{(q)}\otimes\mathcal{H}_{V,+}^{(n-q)})$. □

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