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Expansion of the Many-body quantum Gibbs state of the Bose–Hubbard model on a finite graph

Zied Ammari, Shahnaz Farhat, and Sören Petrat

Abstract. We consider the many-body quantum Gibbs state for the Bose–Hubbard model on a finite graph at positive temperature. We scale the interaction with the inverse temperature, corresponding to a mean-field limit where the temperature is of the order of the average particle number. For this model it is known that the many-body Gibbs state converges, as temperature goes to infinity, to the Gibbs measure of a discrete nonlinear Schrödinger equation, i.e., a Gibbs measure defined in terms of a one-body theory. In this article we extend these results by proving an expansion to any order of the many-body Gibbs state with inverse temperature as a small parameter. The coefficients in the expansion can be calculated as vacuum expectation values using a recursive formula, and we compute the first two coefficients explicitly.

1. Introduction and main result

Within the research field of mathematical physics, proving the validity of effective equations starting from microscopic interacting theories has been a long-standing and active research topic. The mathematical challenge is to prove the convergence of the solution of a very complicated equation to the solution of a much simpler equation in an appropriate scaling regime motivated by physics. The scaling regime is usually such that the effects of the microscopic interaction simplify. For example, in a mean-field type scaling limit this simplification could be achieved through averaging, and for a mathematical rigorous derivation we need to estimate the error coming from replacing the interaction by its mean.

One particular microscopic theory of interest is quantum mechanics, where the corresponding equation in the non-relativistic case is the many-body Schrödinger equation. While this equation is linear, the corresponding effective equations are usually nonlinear but only one-body (or few-body) theories, which makes their analysis much easier and allows, e.g., for numerical solutions. Quantum effects are particularly prominent at low temperature, so much research has been devoted to the low or even zero temperature regimes. Associated effective equations are for example the Hartree, Hartree-Fock, and Gross–Pitaevskii equations; see, e.g., the reviews [4, 26]. On the other hand, high or even infinite temperatures are clearly relevant as well, and here Gibbs states offer a good mathematical framework for studying these regimes; see, e.g., [23].

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In this article, we aim at bringing different approaches in the study of zero and infinite temperature regimes together. For technical simplicity we choose to study the Bose–Hubbard model, which is a lattice model of spinless bosons with on-site interaction that is prominently used in the study of superfluid-insulator phase transitions. We consider a scaling limit where the temperature goes to infinity, the interaction is scaled with the inverse temperature, and the temperature and the average particle number are of the same order. To the best of our knowledge, such a limit was first considered in [20] for finite-dimensional Hilbert spaces. Hence, the inverse average particle number (or inverse temperature) is a small parameter ε, and the system is in a mean-field scaling regime. Within this model it is known (see, e.g., [2]) that the many-body Gibbs state of the Bose–Hubbard model converges to a nonlinear Gibbs measure described by a discrete Hartree functional. In our main result, we prove a much more precise convergence statement, namely an asymptotic expansion of the Gibbs state. Here, the lowest order is the known nonlinear Gibbs measure, while the derivation of all higher orders, to the best of our knowledge, is new.

The motivation for our work comes from three different directions: (1) The recent derivations of nonlinear Gibbs measures from many-body quantum mechanics in a coupled infinite temperature and mean-field limit, (2) The recent proofs of asymptotic expansions for zero-temperature Bose gases in the mean-field limit, (3) The recent results on connecting the quantum and classical Kubo–Martin–Schwinger (KMS) conditions through a coupled high temperature and mean-field limit. Let us explain these motivations in more detail before we introduce our model in Section 1.1, and state our main results in Section 1.2.

(1) The derivation of nonlinear Gibbs measures from many-body quantum mechanics has recently received a lot of attention in the context of the Bose gas with pair interaction in the continuum. For example, in [17, 23, 28] convergence for the partition function and reduced density matrices is proved. In these results the interaction is scaled down with the inverse temperature, analogous to the limit we consider in this article. Note that for continuous systems in two and three dimensions, a renormalization of the nonlinear Gibbs measure is necessary (see [16, 18, 22, 24]), and even its definition via Gaussian measures is non-trivial. In this article, we avoid such technical difficulties associated with continuous systems by considering the simpler Bose–Hubbard model which is defined on a lattice. We furthermore consider only a finite graph instead of an infinite system for technical simplicity. So one motivation for our work is to improve results such as [17, 23, 28] (within our much simpler technical framework) in the sense of proving the validity of an asymptotic expansion compared to only proving the limit.

(2) Another motivation for our work is that such higher order expansions have recently been proved for the continuous Bose gas in the mean-field limit at zero temperature for low-lying eigenvalues and the corresponding (excited and ground) eigenstates [10], and for the dynamics [9, 14]; see also [5, 6] for reviews of these results, and [7, 8] for applications. These results motivated us to prove asymptotic expansions for other relevant scaling limits, such as the coupled mean-field and high temperature limit we consider in this article. At zero temperature and in the mean-field limit, the leading order is described by the

Hartree equation (a nonlinear Schrödinger equation with convolution-type nonlinearity). Note that there are also results concerning the dynamics of discrete nonlinear Schrödinger (DNLS) equations and their derivation from many-body quantum theory, e.g., in [27]. The next-to leading order is described by Bogoliubov theory. The expansion is then proved by using perturbation theory around Bogoliubov theory. In our main result in this article, the Hartree equation appears as well in the limiting Gibbs measure. However, in contrast to the zero-temperature case, we do not see Bogoliubov theory clearly emerging in our high temperature limit.

(3) A further motivation for our work is that recently the Kubo–Martin–Schwinger condition for the thermal equilibrium of quantum and classical systems has attracted some interest [2, 3, 13, 29] (see [1, 15, 19, 21] for older results). In particular, one can interpret the Gibbs measure as the KMS equilibrium state for the discrete nonlinear Schrödinger equation. More generally this concept extends to Hamiltonian systems governed by PDEs (see [3] and references therein). One of the remarkable properties is that the quantum and classical KMS conditions can be linked to each other rigorously through the same high temperature limit that we are considering here. Therefore our expansion of the many-body quantum Gibbs state provides information on the KMS condition as well. We briefly describe here this relation and refer the reader to [2] for more details. The Bose–Hubbard model defines a dynamical system $(\alpha_t, \omega_\varepsilon)$ given by a group of automorphisms over the algebra of bounded operators,

$$\alpha_t(A) = e^{i\frac{t}{\varepsilon}H_\varepsilon}\, A\, e^{-i\frac{t}{\varepsilon}H_\varepsilon},$$

where H_ε is the Bose–Hubbard Hamiltonian defined in (1.4), and by a quantum Gibbs state defined by

$$\omega_\varepsilon(A) = \frac{\mathrm{Tr}(e^{-\beta H_\varepsilon}A)}{\mathrm{Tr}(e^{-\beta H_\varepsilon})}.$$

It is known that the Gibbs state ω_ε is the unique KMS state at inverse temperature $\varepsilon\beta$ of the Bose–Hubbard system satisfying

$$\omega_\varepsilon\big(A\,\alpha_{i\varepsilon\beta}(B)\big) = \omega_\varepsilon(BA), \tag{1.1}$$

where $\alpha_{i\varepsilon\beta}$ is an analytic extension of the dynamics to complex times. A specific choice of observables in (1.1) leads to

$$\omega_\varepsilon\left(W_\varepsilon(f)\,\frac{\alpha_{i\varepsilon\beta}\big(W_\varepsilon(g)\big) - W_\varepsilon(g)}{i\varepsilon}\right) = \omega_\varepsilon\left(\frac{\big[W_\varepsilon(g), W_\varepsilon(f)\big]}{i\varepsilon}\right), \tag{1.2}$$

where $W_\varepsilon(\cdot)$ are the Weyl operators in (1.7). According to [2], taking the high temperature limit ($\varepsilon \to 0$) in the relation (1.2) yields the classical KMS condition studied by G. Gallavotti and E. Verboven [19],

$$\beta\int_{\ell^2(G)} e^{i\Re e\langle f,u\rangle}\big\{e^{i\Re e\langle g,u\rangle}, h(u)\big\}\, d\mu_\beta(u) = \int_{\ell^2(G)} \big\{e^{i\Re e\langle g,u\rangle}, e^{i\Re e\langle f,u\rangle}\big\}\, d\mu_\beta(u), \tag{1.3}$$

where $f, g \in \ell^2(G)$, h is the Hamiltonian of the DNLS equation in (1.9), μ_β is the Gibbs measure, and $\{\cdot,\cdot\}$ is the Poisson bracket. Hence our main Theorem 1.1 provides an optimal rate of convergence and an expansion of both sides of (1.2) in terms of the inverse temperature parameter.

Finally, let us mention another outlook on the topic of this article, namely the relationship with entropy and with Berezin quantization on symplectic manifolds. In fact, the Gibbs state and respectively the Gibbs measure are minimizers of their corresponding von Neumann and Boltzmann entropies, so that we can approach the high temperature limit in terms of these variational problems (see [23]). On the other hand, the high temperature limit can be interpreted as a classical limit for Gibbs states in the framework of deformation quantization (see, e.g., [12, 29]). Such a problem was recently studied in [29] and a convergence (to the leading order without expansion) similar to our result is proved in [29, Proposition 3.3]. The argument is based on Berezin–Lieb and Peierls–Bogoliubov inequalities [25]. It would be interesting to apply our method to these two approaches.

1.1. General framework

Let $G = (V, E)$ be a finite (undirected and simple) graph, with V the set of vertices and E the set of edges. The degree of a vertex $x \in V$ is denoted by $\deg(x)$. We consider the one-body (complex) Hilbert space $\ell^2(G)$, endowed with the standard scalar product and norm

$$\langle u, v\rangle = \sum_{x\in V} \overline{u(x)}v(x), \quad \|u\| = \Big(\sum_{x\in V} \big|u(x)\big|^2\Big)^{1/2}.$$

We will sometimes use the orthonormal basis $\{e_x\}_{x\in V}$ of $\ell^2(G)$ defined by

$$e_x(y) = \delta_{xy}, \quad \forall y \in V.$$

The symmetric Fock space $\mathcal{F}$ is defined as

$$\mathcal{F} := \Gamma\big(\ell^2(G)\big) = \bigoplus_{m\geq 0} \ell^2(G)^{\otimes_s^m} \simeq \bigoplus_{m\geq 0} \ell_s^2(G^m),$$

where $\otimes_s$ denotes the symmetric tensor product, and $\ell_s^2(G^m)$ is the symmetric ℓ^2 space over G^m. Let a_x^* and a_x be the usual creation and annihilation operators satisfying the canonical commutation relations

$$[a_x, a_y^*] = \delta_{xy}, \quad [a_x, a_y] = 0 = [a_x^*, a_y^*],$$

and set, for any $u \in \ell^2(G)$,

$$a^*(u) = \sum_{x\in V} u(x)\, a_x^*, \quad a(u) = \sum_{x\in V} \overline{u(x)}\, a_x.$$

The second quantization of an operator B on $\ell^2(G)$ with matrix elements $B_{xy} = \langle e_x, Be_y\rangle$ is defined as

$$\mathrm{d}\Gamma(B) := \sum_{x,y\in V} a_x^* B_{xy} a_y,$$

and we define the number operator as

$$\mathcal{N} := \mathrm{d}\Gamma(\mathbb{1}) = \sum_{x\in V} a_x^* a_x.$$

For any small parameter $\varepsilon > 0$, coupling constant $\lambda > 0$, and chemical potential $\kappa < 0$, we define the Bose–Hubbard Hamiltonian on $\mathcal{F}$ as

$$H_\varepsilon := \frac{\varepsilon}{2} \sum_{x,y\in V, x\sim y} (a_x^* - a_y^*)(a_x - a_y) - \varepsilon\kappa \sum_{x\in V} a_x^* a_x + \varepsilon^2 \frac{\lambda}{2} \sum_{x\in V} a_x^* a_x^* a_x a_x, \quad (1.4)$$

where $x \sim y$ means that x and y are nearest neighbors. Note that by introducing the discrete Laplacian Δ_d as

$$(\Delta_d u)(x) := -\deg(x) u(x) + \sum_{y\in V, y\sim x} u(y),$$

we can rewrite the Bose–Hubbard Hamiltonian as

$$H_\varepsilon = \varepsilon \mathrm{d}\Gamma(-\Delta_d - \kappa\mathbb{1}) + \varepsilon^2 \frac{\lambda}{2} \sum_{x\in V} a_x^* a_x^* a_x a_x. \quad (1.5)$$

1.2. Main result

The Gibbs state ω_ε at inverse temperature $\beta > 0$ is defined as

$$\omega_\varepsilon(A) := \frac{1}{Z_\varepsilon} \mathrm{Tr}(e^{-\beta H_\varepsilon} A) \quad (1.6)$$

for any operator A on $\mathcal{F}$, where $Z_\varepsilon := \mathrm{Tr}(e^{-\beta H_\varepsilon})$ is the partition function. Note that $Z_\varepsilon < \infty$ since we chose $\kappa < 0$, see, e.g., [11, Proposition 5.2.27]. We will keep the inverse temperature as a fixed parameter, and instead consider ε as the small parameter, so the limit $\varepsilon \to 0$ corresponds to a limit where the inverse temperature and the coupling constant each go to zero in the same way. Our goal is to expand ω_ε in powers of ε. In order to write down such a series expansion concretely, let us consider a Weyl operator with the right semiclassical structure. For any $f \in \ell^2(G)$ the Weyl operator $W_\varepsilon(f)$ is defined as

$$W_\varepsilon(f) := e^{i\sqrt{\varepsilon}\Phi(f)}, \quad \text{with } \Phi(f) := \frac{1}{\sqrt{2}}\big(a(f) + a^*(f)\big). \quad (1.7)$$

In our main result Theorem 1.1 we prove an expansion for

$$Z_\varepsilon\, \omega_\varepsilon\big(W_\varepsilon(f)\big) = \mathrm{Tr}\left(e^{-\beta H_\varepsilon} W_\varepsilon(f)\right). \quad (1.8)$$

Note that for $f = 0$ this implies an expansion for Z_ε, and both results together can be combined into a single expansion for $\omega_\varepsilon(W_\varepsilon(f))$, see Remark 1.2. Note, however, that in the limit $\varepsilon \to 0$ both quantities diverge like $c_\varepsilon := (\varepsilon\pi)^{-|V|}$, therefore we write down the expansion for $c_\varepsilon^{-1}\operatorname{Tr}(e^{-\beta H_\varepsilon} W_\varepsilon(f))$. The expansion could also be written down, e.g., for reduced one-particle density matrices, see Remark 1.3.

The leading order in the expansion is a classical Gibbs measure, defined in terms of the Hamiltonian of the discrete nonlinear Schrödinger equation

$$h(u) := \langle u, (-\Delta_d)u\rangle - \kappa\|u\|^2 + \frac{\lambda}{2}\sum_{x\in V}|u(x)|^4. \tag{1.9}$$

We introduce the corresponding nonlinear Hartree operator h^{H} as

$$h^{\mathrm{H}}(u) := -\Delta_d u - \kappa u + \lambda|u|^2 u. \tag{1.10}$$

The Gibbs measure is defined as

$$d\mu_\beta(u) = \frac{1}{z_\beta} e^{-\beta h(u)}\mathrm{d}u, \tag{1.11}$$

where $\mathrm{d}u = \prod_{x\in V}\mathrm{d}u_x$ with $\mathrm{d}u_x$ the Lebesgue measure on $\mathbb{C}$, and $z_\beta = \int_{\ell^2(G)} e^{-\beta h(u)}\,\mathrm{d}u$. In our setting it is known that

$$\lim_{\varepsilon\to 0}\omega_\varepsilon\big(W_\varepsilon(f)\big) = \int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle}\,d\mu_\beta(u),$$

see, e.g., [2]. To expand $c_\varepsilon^{-1}\operatorname{Tr}(e^{-\beta H_\varepsilon} W_\varepsilon(f))$, we employ an explicit resolution of the identity using a coherent state $\widetilde{W}_\varepsilon(u)|\Omega\rangle$, where $|\Omega\rangle$ represents the vacuum state and $\widetilde{W}_\varepsilon(u)$ is the rescaled Weyl operator as defined in (1.14). Inserting this resolution of identity into $c_\varepsilon^{-1}\operatorname{Tr}(e^{-\beta H_\varepsilon} W_\varepsilon(f))$ transforms the expression into an integral involving the vacuum expectation of the product of $e^{-\beta\widetilde{W}_\varepsilon(u)^* H_\varepsilon \widetilde{W}_\varepsilon(u)}$ and $\widetilde{W}_\varepsilon(u)^* W_\varepsilon(f)\widetilde{W}_\varepsilon(u)$. By applying the shifting properties of the Weyl operators, we can rewrite the first term as

$$e^{-\beta\widetilde{W}_\varepsilon(u)^* H_\varepsilon \widetilde{W}_\varepsilon(u)} = e^{-\beta h(u)} e^{-\beta A_\varepsilon(u)}$$

where $A_\varepsilon(u)$ is an ε-dependent Wick polynomial defined in (2.2)–(2.3). Hence when taking vacuum expectations, we can apply a Taylor expansion to $e^{-\beta A_\varepsilon(u)}$, which reduces the problem to evaluating the ε-dependent terms $A_\varepsilon(u)^m|\Omega\rangle$. Such terms can then be reordered by Wick's Theorem and expanded as a power series on ε, with $A_\ell^m(u)$ as the resulting coefficients that are defined by the recursive formula in (2.8).

Our main result is the following.

Theorem 1.1 (Higher order expansion). *For any $N\in\mathbb{N}$, $f\in\ell^2(G)$, and $\varepsilon>0$ small enough, we have*

$$\begin{aligned}(\varepsilon\pi)^{|V|}&\operatorname{Tr}\big(e^{-\beta H_\varepsilon} W_\varepsilon(f)\big)\\ &= \sum_{j=0}^{N}\varepsilon^j\int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle} C_j(u,f)e^{-\beta h(u)}\mathrm{d}u + \mathcal{O}(\varepsilon^{N+1}),\end{aligned}$$

where the $\mathcal{O}(\varepsilon^{N+1})$ *term may depend on* f *and the parameters* β, κ, *and* λ. *The coefficients* C_j *are* ε*-independent and given as* $C_0(u, f) \equiv 1$, *and, for* $j \geq 1$,

$$C_j(u, f) = \frac{(-1)^j}{j!\,4^j} \|f\|^{2j} + \sum_{m=1}^{2j} \frac{(-\beta)^m}{m!} \sum_{\ell=m}^{\min(4m-2,2j)} \frac{i^{2j-\ell}}{(2j-\ell)!} \big\langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{2j-\ell}\Omega\big\rangle, \quad (1.12)$$

where Ω *is the vacuum in* $\mathcal{F}$ *and* $A_\ell^{(m)}(u)$ *are defined by the recursive formula in* (2.8). *In particular,*

$$C_1(u, f) = -\frac{\|f\|^2}{4} - i\frac{\beta}{\sqrt{2}}\langle h^{\mathrm{H}}(u), f\rangle + \frac{\beta^2}{2}\left\|h^{\mathrm{H}}(u)\right\|^2 \quad (1.13)$$

and $C_2(u, f)$ *is given in the appendix.*

The theorem is proved in Section 3.

Remark 1.2. Note that for $f = 0$ we have

$$C_j(u, 0) = \sum_{m=\lceil \frac{1}{2}(j+1)\rceil}^{2j} \frac{(-\beta)^m}{m!} \big\langle A_{2j}^{(m)}(u)\Omega, \Omega\big\rangle,$$

which are the coefficients in the expansion of $(\varepsilon\pi)^{|V|} Z_\varepsilon$. Combining both expansions

$$(\varepsilon\pi)^{|V|}\,\mathrm{Tr}\left(e^{-\beta H_\varepsilon} W_\varepsilon(f)\right) = \sum_{j=0}^{N} \varepsilon^j\, \widetilde{C}_j(f) + \mathcal{O}(\varepsilon^{N+1}),$$

$$(\varepsilon\pi)^{|V|}\,\mathrm{Tr}(e^{-\beta H_\varepsilon}) = \sum_{j=0}^{N} \varepsilon^j\, \widetilde{C}_j(0) + \mathcal{O}(\varepsilon^{N+1}),$$

where $\widetilde{C}_0(0) = z_\beta$, leads to an expansion of the Gibbs state. Denoting by $\alpha \in \mathbb{N}^k$ a multi-index with $|\alpha| := \sum_{i=1}^k \alpha_i$, we find

$$\begin{aligned}
&\omega_\varepsilon\big(W_\varepsilon(f)\big) \\
&= \frac{\widetilde{C}_0(f)}{z_\beta} + \sum_{j=1}^{N} \varepsilon^j \left[\sum_{\ell=0}^{j-1} \frac{\widetilde{C}_\ell(f)}{z_\beta} \sum_{k=1}^{j-\ell} \sum_{\substack{\alpha\in\mathbb{N}^k \\ |\alpha|=j-\ell}} \prod_{m=1}^{k} \left(-\frac{\widetilde{C}_{\alpha_m}(0)}{z_\beta}\right) + \frac{\widetilde{C}_j(f)}{z_\beta}\right] + \mathcal{O}(\varepsilon^{N+1}) \\
&= \int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle} \frac{e^{-\beta h(u)}\mathrm{d}u}{z_\beta} \\
&\quad + \varepsilon \int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle} \left[-\frac{\|f\|^2}{4} - i\frac{\beta}{\sqrt{2}}\langle h^{\mathrm{H}}(u), f\rangle + \frac{\beta^2}{2}\left\|h^{\mathrm{H}}(u)\right\|^2\right] \frac{e^{-\beta h(u)}}{z_\beta}\mathrm{d}u \\
&\quad - \varepsilon\left[\int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle} \frac{e^{-\beta h(u)}}{z_\beta}\mathrm{d}u\right]\left[\int_{\ell^2(G)} \frac{\beta^2}{2}\left\|h^{\mathrm{H}}(u)\right\|^2 \frac{e^{-\beta h(u)}}{z_\beta}\mathrm{d}u\right] + \mathcal{O}(\varepsilon^2).
\end{aligned}$$

Remark 1.3. Note that we could also provide an expansion for expectations of other operators than the Weyl operator $W_\varepsilon(f)$, e.g., for the reduced one-particle density matrix

$$\mathrm{Tr}(e^{-\beta H_\varepsilon}\varepsilon a_x^* a_y).$$

For this example the expansion reads

$$\begin{aligned}(\varepsilon\pi)^{|V|}&\,\mathrm{Tr}(e^{-\beta H_\varepsilon}\varepsilon a_x^* a_y)\\ &= \int_{\ell^2(G)} \bar{u}_x\, u_y\, e^{-\beta h(u)}\mathrm{d}u\\ &\quad + \varepsilon\int_{\ell^2(G)}\Big[\frac{\beta^2}{2}\bar{u}_x\, u_y \big\|h^{\mathrm{H}}(u)\big\|^2 - \beta u_y\big\langle h^{\mathrm{H}}(u),\, e_x\big\rangle\Big]e^{-\beta h(u)}\mathrm{d}u + \mathcal{O}(\varepsilon^2).\end{aligned}$$

Remark 1.4. Let us note that extending our result to an infinite lattice or to the continuous case presents significant challenges. For example, we immediately notice that when the size $|V|$ becomes infinite, the normalization $(\varepsilon\pi)^{|V|}$ diverges. Hence, the resolution of identity in such infinite-dimensional spaces is non-trivial and cannot be directly computed as in (1.16) below. Moreover, in infinite-dimensional spaces, the formal measure $\mathrm{d}u$ in the definition of the nonlinear Gibbs measure μ_β in (1.11) cannot be defined using the Lebesgue measure. Instead, one should use Gaussian measures on infinite-dimensional Hilbert spaces, for example the space $L^2(\mathbb{T}^d)$ on the d-dimensional torus $\mathbb{T}^d$. Furthermore, even in this framework, the construction of Gibbs measures is non-trivial in dimension $d = 2$ and $d = 3$, since the Gaussian measures concentrate on distributions and a renormalization of the nonlinear term of the Schrödinger equation is required.

1.3. Notation and summary of proof

In addition to the Weyl operator

$$W_\varepsilon(f) = e^{i\sqrt{\frac{\varepsilon}{2}}(a(f)+a^*(f))},$$

from (1.7), let us introduce the rescaled Weyl operator

$$\widetilde{W}_\varepsilon(u) := e^{\frac{1}{\sqrt{\varepsilon}}(a^*(u)-a(u))}. \tag{1.14}$$

With the latter we define the coherent state

$$|u_\varepsilon\rangle := \widetilde{W}_\varepsilon(u)|\Omega\rangle = e^{-\frac{\|u\|^2}{2\varepsilon}}\, e^{\frac{1}{\sqrt{\varepsilon}}a^*(u)}|\Omega\rangle, \tag{1.15}$$

where $|\Omega\rangle$ is the vacuum in $\mathcal{F}$, and the equality follows from the Baker–Campbell–Hausdorff formula. Then, by direct computation on the finite graph G, we have the resolution of identity

$$c_\varepsilon \int_{\ell^2(G)} |u_\varepsilon\rangle\,\langle u_\varepsilon|\mathrm{d}u = 1, \tag{1.16}$$

where $c_\varepsilon := (\varepsilon\pi)^{-|V|}$. It is important to note that such a resolution of identity is not valid in infinite-dimensional spaces as already highlighted in Remark 1.4. This presents a significant challenge when attempting to generalize our results to continuum cases. The idea of the proof is to insert the identity (1.16) in the computation of $\mathrm{Tr}(e^{-\beta H_\varepsilon} W_\varepsilon(f))$, so that it only contains $\widetilde{W}_\varepsilon(u)^* H_\varepsilon \widetilde{W}_\varepsilon(u)$ instead of H_ε directly. This Weyl-transformed Hamiltonian can be written as

$$\widetilde{W}_\varepsilon(u)^* H_\varepsilon \widetilde{W}_\varepsilon(u) = h(u) + \sum_{j=1}^{4} \varepsilon^{j/2} A_j(u), \tag{1.17}$$

for some ε-independent operators $A_j(u)$, see Section 2.1. It remains to expand the exponential of (1.17), and $W_\varepsilon(f)$, in powers of ε. This is done in Section 2.2 where we compute the coefficients of the expansion and thus define the remainder terms. In Section 3 we prove Theorem 1.1 by estimating the remainder terms. Finally, we explicitly compute the first two coefficients of the expansion in the appendix.

Notation. In the following sections, we use in our estimates constants C that may depend on the parameters of our model, and that can be different from line to line.

2. Formal expansion

2.1. Resolution of identity

First, we insert the resolution of identity (1.16) into the computation of $\mathrm{Tr}(e^{-\beta H_\varepsilon} W_\varepsilon(f))$.

Lemma 2.1 (Integral formula). *We have*

$$\frac{1}{c_\varepsilon} \mathrm{Tr}\left(e^{-\beta H_\varepsilon} W_\varepsilon(f)\right) = \int_{\ell^2(G)} e^{\sqrt{2} i \Re e \langle f, u\rangle} \left\langle \Omega, e^{-\beta A_\varepsilon(u)} W_\varepsilon(f) \Omega \right\rangle e^{-\beta h(u)} \mathrm{d}u, \tag{2.1}$$

where $W_\varepsilon(\cdot)$ is the Weyl operator defined in (1.7), and

$$A_\varepsilon(u) := \sum_{j=1}^{4} \varepsilon^{j/2} A_j(u) \tag{2.2}$$

with

$$\begin{aligned}
A_1(u) &:= a^*\big(h^{\mathrm{H}}(u)\big) + a\big(h^{\mathrm{H}}(u)\big), \\
A_2(u) &:= \mathrm{d}\Gamma(-\Delta_d) - \kappa \mathcal{N} + \frac{\lambda}{2} \sum_{x\in V} \big(a_x^* a_x^* u_x^2 + 4 a_x^* a_x |u_x|^2 + a_x a_x \bar{u}_x^2\big), \\
A_3(u) &:= \frac{\lambda}{2} \sum_{x\in V} (a_x^* a_x^* a_x u_x + a_x^* a_x a_x \bar{u}_x), \\
A_4(u) &:= \frac{\lambda}{2} \sum_{x\in V} a_x^* a_x^* a_x a_x.
\end{aligned} \tag{2.3}$$

Proof. We use the resolution of identity (1.16) to expand

$$\begin{aligned}\frac{1}{c_\varepsilon}\operatorname{Tr}\big(e^{-\beta H_\varepsilon}W_\varepsilon(f)\big) &= \int_{\ell^2(G)} \big\langle u_\varepsilon,\, e^{-\beta H_\varepsilon}\, W_\varepsilon(f)\, u_\varepsilon\big\rangle \mathrm{d}u \\ &= \int_{\ell^2(G)} \big\langle \Omega,\, \widetilde{W}_\varepsilon(u)^* e^{-\beta H_\varepsilon}\widetilde{W}_\varepsilon(u)\, \widetilde{W}_\varepsilon(u)^*\, W_\varepsilon(f)\widetilde{W}_\varepsilon(u)\,\Omega\big\rangle \mathrm{d}u \\ &= \int_{\ell^2(G)} \big\langle \Omega,\, e^{-\beta \widetilde{W}_\varepsilon(u)^* H_\varepsilon \widetilde{W}_\varepsilon(u)}\, \widetilde{W}_\varepsilon(u)^*\, W_\varepsilon(f)\, \widetilde{W}_\varepsilon(u)\Omega\big\rangle \mathrm{d}u.\end{aligned}$$

To expand the above expression in powers of ε, we use the shifting properties of the Weyl operator, i.e.,

$$\begin{aligned}\widetilde{W}_\varepsilon(u)^*\, a_x^*\, \widetilde{W}_\varepsilon(u) &= a_x^* + \frac{1}{\sqrt{\varepsilon}}\overline{u(x)}, \\ \widetilde{W}_\varepsilon(u)^*\, a_x\, \widetilde{W}_\varepsilon(u) &= a_x + \frac{1}{\sqrt{\varepsilon}}u(x),\end{aligned} \tag{2.4}$$

$$\begin{aligned}\widetilde{W}_\varepsilon(u)^*\, a^*(f)\, \widetilde{W}_\varepsilon(u) &= a^*(f) + \frac{1}{\sqrt{\varepsilon}}\langle u, f\rangle, \\ \widetilde{W}_\varepsilon(u)^*\, a(f)\, \widetilde{W}_\varepsilon(u) &= a(f) + \frac{1}{\sqrt{\varepsilon}}\langle f, u\rangle.\end{aligned} \tag{2.5}$$

Using (2.4) gives us directly (1.17) with the coefficients (2.3). Furthermore, using (2.5), we get

$$\widetilde{W}_\varepsilon(u)^*\, W_\varepsilon(f)\, \widetilde{W}_\varepsilon(u) = e^{i\sqrt{\frac{\varepsilon}{2}}\,\widetilde{W}_\varepsilon(u)^*(a^*(f)+a(f))\widetilde{W}_\varepsilon(u)} = e^{\sqrt{2}i\,\Re e\langle f,u\rangle}\, W_\varepsilon(f),$$

which proves (2.1). ■

2.2. Taylor expansion

In order to expand the right-hand side of (2.1), let us write down the Taylor expansions with remainders for $e^{-\beta A_\varepsilon(u)}$ and $W_\varepsilon(f)$. For given $N \in \mathbb{N}$, we have

$$e^{-\beta A_\varepsilon(u)} = \underbrace{\sum_{m=0}^{N} \frac{\big(-\beta A_\varepsilon(u)\big)^m}{m!}}_{=:\mathcal{M}_A^{(N)}} + \underbrace{\big(-\beta A_\varepsilon(u)\big)^{N+1}\int_0^1 e^{-s\beta A_\varepsilon(u)}\frac{(1-s)^N}{N!}\mathrm{d}s}_{=:\mathcal{R}_A^{(N)}}, \tag{2.6a}$$

$$W_\varepsilon(f) = \underbrace{\sum_{n=0}^{N} \varepsilon^{\frac{n}{2}}\frac{\big(i\Phi(f)\big)^n}{n!}}_{=:\mathcal{M}_f^{(N)}} + \underbrace{\big(i\sqrt{\varepsilon}\Phi(f)\big)^{N+1}\int_0^1 e^{is\sqrt{\varepsilon}\Phi(f)}\frac{(1-s)^N}{N!}\mathrm{d}s}_{=:\mathcal{R}_f^{(N)}}. \tag{2.6b}$$

The above formulas make sense by functional calculus. Note that (2.6a) is not an expansion in powers of $\sqrt{\varepsilon}$ yet because $A_\varepsilon(u)$ contains different powers of $\sqrt{\varepsilon}$. Furthermore, according to (2.1), we only need to evaluate $(A_\varepsilon(u))^m$ acting on the vacuum Ω. Recall that Ω is an analytic vector of the field operator $\Phi(f)$ and it is in the domain of any Wick monomial. Ordering $(A_\varepsilon(u))^m|\Omega\rangle$ in powers of $\sqrt{\varepsilon}$ gives, for $m > 0$,

$$A_\varepsilon(u)^m|\Omega\rangle = \sum_{\ell=m}^{4m-2} \varepsilon^{\frac{\ell}{2}} A_\ell^{(m)}(u)|\Omega\rangle, \tag{2.7}$$

where $A_\ell^{(m)}(u)$ is given by

$$\begin{aligned} A_\ell^{(m)} &= A_1^{(1)} A_{\ell-1}^{(m-1)} + A_2^{(1)} A_{\ell-2}^{(m-1)} + A_3^{(1)} A_{\ell-3}^{(m-1)} + A_4^{(1)} A_{\ell-4}^{(m-1)} \\ &= \sum_{\substack{\alpha\in\{1,2,3,4\}^m \\ |\alpha|=\ell}} \prod_{k=1}^m A_{\alpha_k}, \end{aligned} \tag{2.8}$$

where the $A_{\alpha_k}(u) \equiv A_{\alpha_k}^{(1)}(u)$ for $\alpha_k \in \{1,2,3,4\}$ are given in Lemma 2.1. Here, we have used the multi-index notation, i.e., $|\alpha| = \sum_{k=1}^m \alpha_k$. Note that in (2.7) the $\ell = 4m-1$ and $\ell = 4m$ terms vanish since both $A_3(u)$ and $A_4(u)$ contain an a_x acting on the vacuum $|\Omega\rangle$. For later convenience we define $A_\ell^{(m)}(u)$ to be zero outside the range of indices in (2.7). To summarize, for any $\ell \in \mathbb{N}$,

$$A_\ell^{(m)}(u) := \begin{cases} 0, & \text{for } \ell < m \text{ or } \ell > 4m-2, \\ (2.8), & \text{otherwise.} \end{cases} \tag{2.9}$$

We can now state the expansion of the term $\langle e^{-\beta A_\varepsilon(u)}\Omega, W_\varepsilon(f)\Omega\rangle$ from (2.1) in powers of $\sqrt{\varepsilon}$.

Lemma 2.2 (Formal expansion). *For any $N \in \mathbb{N}$ we have*

$$\left\langle e^{-\beta A_\varepsilon(u)}\Omega, W_\varepsilon(f)\Omega\right\rangle = \sum_{j=0}^N \varepsilon^{\frac{j}{2}} C_{\frac{j}{2}}(u,f) + R_\varepsilon^{(N)}(u,f), \tag{2.10}$$

with $C_0(u,f) \equiv 1$ and where, for $j \geq 1$,

$$\begin{aligned} C_{\frac{j}{2}}(u,f) := {}& \frac{i^j}{j!}\left\langle\Omega, \Phi(f)^j\Omega\right\rangle \\ &+ \sum_{m=1}^j \frac{(-\beta)^m}{m!} \sum_{\ell=m}^{\min(4m-2,j)} \frac{i^{j-\ell}}{(j-\ell)!}\left\langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{j-\ell}\Omega\right\rangle, \end{aligned} \tag{2.11}$$

with $A_\ell^{(m)}(u)$ as defined in (2.9). The remainder term $R_\varepsilon^{(N)}(u,f)$ is given as

$$R_\varepsilon^{(N)}(u,f) := \left\langle\Omega, \left(\mathcal{R}_{f,A}^{(N)} + \mathcal{M}_A^{(N)}\mathcal{R}_f^{(N)} + \mathcal{R}_A^{(N)}\mathcal{M}_f^{(N)} + \mathcal{R}_A^{(N)}\mathcal{R}_f^{(N)}\right)\Omega\right\rangle, \tag{2.12}$$

with $\mathcal{M}_A^{(N)}$, $\mathcal{R}_A^{(N)}$, $\mathcal{M}_f^{(N)}$, *and* $\mathcal{R}_f^{(N)}$ *from* (2.6), *and*

$$\mathcal{R}_{f,A}^{(N)} := \sum_{j=N+1}^{5N-2} \varepsilon^{\frac{j}{2}} \sum_{m=1}^{j} \frac{(-\beta)^m}{m!} \sum_{\ell=\max(m,j-N)}^{\min(4m-2,j)} \frac{i^{j-\ell}}{(j-\ell)!} \langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{j-\ell}\Omega\rangle.$$

Proof. By using the Taylor expansions (2.6a) and (2.6b) we have

$$\begin{aligned}&\langle e^{-\beta A_\varepsilon(u)}\Omega, W_\varepsilon(f)\Omega\rangle\\ &\quad = \langle \Omega, \mathcal{M}_A^{(N)}\mathcal{M}_f^{(N)}\Omega\rangle + \langle \Omega, (\mathcal{M}_A^{(N)}\mathcal{R}_f^{(N)} + \mathcal{R}_A^{(N)}\mathcal{M}_f^{(N)} + \mathcal{R}_A^{(N)}\mathcal{R}_f^{(N)})\Omega\rangle.\end{aligned}$$

It remains to multiply out the first term in the expression above. Defining $a_m = (-\beta)^m/m!$ and $b_n = i^n/n!$ we have

$$\begin{aligned}\langle \Omega, \mathcal{M}_A^{(N)}\mathcal{M}_f^{(N)}\Omega\rangle &= \sum_{m=0}^{N}\sum_{n=0}^{N} \varepsilon^{\frac{n}{2}} a_m b_n \langle A_\varepsilon(u)^m\Omega, \Phi(f)^n\Omega\rangle\\ &= \sum_{n=0}^{N} \varepsilon^{\frac{n}{2}} b_n \langle \Omega, \Phi(f)^n\Omega\rangle\\ &\quad + \sum_{m=1}^{N}\sum_{n=0}^{N}\sum_{p=m}^{4m-2} \varepsilon^{\frac{p+n}{2}} a_m b_n \langle A_p^{(m)}(u)\Omega, \Phi(f)^n\Omega\rangle.\end{aligned}$$

It is now convenient to use the convention (2.9), i.e., $A_\ell^{(m)}(u) := 0$ for $\ell < m$ or $\ell > 4m-2$, since then we can rearrange

$$\begin{aligned}&\sum_{m=1}^{N}\sum_{n=0}^{N}\sum_{p=m}^{4m-2} \varepsilon^{\frac{p+n}{2}} a_m b_n \langle A_p^{(m)}(u)\Omega, \Phi(f)^n\Omega\rangle\\ &\quad = \sum_{p=0}^{\infty}\sum_{n=0}^{N}\sum_{m=1}^{N} \varepsilon^{\frac{p+n}{2}} a_m b_n \langle A_p^{(m)}(u)\Omega, \Phi(f)^n\Omega\rangle\\ &\quad = \sum_{j=0}^{\infty} \varepsilon^{\frac{j}{2}} \sum_{\tilde\ell=0}^{N}\sum_{m=1}^{N} a_m b_{\tilde\ell} \langle A_{j-\tilde\ell}^{(m)}(u)\Omega, \Phi(f)^{\tilde\ell}\Omega\rangle\\ &\quad = \sum_{j=1}^{5N-2} \varepsilon^{\frac{j}{2}} \sum_{m=1}^{j}\sum_{\tilde\ell=0}^{N} a_m b_{\tilde\ell} \langle A_{j-\tilde\ell}^{(m)}(u)\Omega, \Phi(f)^{\tilde\ell}\Omega\rangle\\ &\quad = \sum_{j=1}^{5N-2} \varepsilon^{\frac{j}{2}} \sum_{m=1}^{j}\sum_{\ell=\max(m,j-N)}^{\min(j,4m-2)} a_m b_{j-\ell} \langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{j-\ell}\Omega\rangle,\end{aligned}$$

renaming $\tilde\ell = j - \ell$ in the last step (and using the convention (2.9) again). In total, this implies the expansion (2.10), noting that $\max(m, j-N) = m$ for $j \le N$ and $m \ge 1$. ■

The expansion from Lemma 2.2 can be simplified by noting that the $\varepsilon^{\frac{j}{2}}$ terms vanish for j odd.

Lemma 2.3 (Vanishing of odd terms). *For all j odd, $C_{\frac{j}{2}}(u, f) = 0$.*

Proof. Recall from (2.8) that

$$A_\ell^{(m)} = \sum_{\substack{\alpha \in \{1,2,3,4\}^m \\ |\alpha| = \ell}} \prod_{k=1}^{m} A_{\alpha_k}.$$

Now recall from the definition (2.3) that each term in A_{α_k} contains exactly α_k creation or annihilation operators (in normal order). Hence, for $|\alpha| = \ell$, the products $\prod_{k=1}^m A_{\alpha_k}$ contain an even (resp. odd) number of creation/annihilation operators for ℓ even (resp. odd). Note that the terms in the products $\prod_{k=1}^m A_{\alpha_k}$ are not necessarily normal ordered, but normal ordering does not change the parity of the number of creation/annihilation operators. In the same way, $\Phi(f)^{j-\ell}$ contains only terms with an even (resp. odd) number of creation/annihilation operators for $0 \leq j - \ell$ even (resp. odd). Since vacuum expectations of terms with an odd number of creation/annihilation operators vanish, we have that

$$\left\langle \Omega, \Phi(f)^j \Omega \right\rangle = 0 = \left\langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{j-\ell}\Omega \right\rangle \quad \text{for } j \text{ odd}$$

and any $0 \leq \ell \leq j$, $1 \leq m \leq j$. Thus, all terms in the definition (2.11) of $C_{\frac{j}{2}}(u, f)$ vanish for j odd. ∎

Lastly, let us compute the first term of $C_{\frac{j}{2}}(u, f)$ explicitly.

Lemma 2.4. *For the first term in (2.11) we find*

$$\frac{i^{2k}}{(2k)!}\left\langle \Omega, \Phi(f)^{2k}\Omega \right\rangle = \frac{(-1)^k}{k!\,4^k}\|f\|^{2k}$$

for any $k \in \mathbb{N}$.

Proof. Such identity is well known and the expression can easily be verified inductively. Alternatively, note that by the Baker–Campbell–Hausdorff formula

$$\sum_{k \geq 0} \frac{1}{(2k)!}\left\langle \Omega, \left(a(f) + a^*(f)\right)^{2k}\Omega \right\rangle$$
$$= \left\langle \Omega, e^{a(f)+a^*(f)}\Omega \right\rangle = e^{\frac{\|f\|^2}{2}} = \sum_{k \geq 0} \frac{\|f\|^{2k}}{2^k\, k!},$$

so comparing coefficients leads to

$$\frac{i^{2k}}{(2k)!}\left\langle \Omega, \Phi(f)^{2k}\Omega \right\rangle = \frac{(-1)^k}{(2k)!} 2^{-k} \frac{(2k)!}{2^k\, k!}\|f\|^{2k} = \frac{(-1)^k}{k!\,4^k}\|f\|^{2k}.$$ ∎

3. Proof of the main result

3.1. Preparatory estimates

The following lemmas will be used to estimate the remainder terms in the expansion of the right-hand side of (2.1). Recall that in our Hamiltonian (1.4) we used the chemical potential $\kappa < 0$, and recall that we defined the coherent state u_ε in (1.15).

Lemma 3.1. *There is α with $0 < \alpha < -\kappa$ such that*

$$\langle u_\varepsilon, e^{-\beta H_\varepsilon} u_\varepsilon \rangle \le e^{-\beta\alpha\|u\|^2} \tag{3.1}$$

for all ε small enough.

Proof. Note that we can write the Hamiltonian (1.4) as $H_\varepsilon = \tilde{H}_\varepsilon - \kappa\varepsilon\mathcal{N}$, with $\tilde{H}_\varepsilon \ge 0$, $-\kappa > 0$ and $[\tilde{H}_\varepsilon, \mathcal{N}] = 0$ in the strong sense. Therefore,

$$\langle u_\varepsilon, e^{-\beta H_\varepsilon} u_\varepsilon \rangle = \langle u_\varepsilon, e^{-\beta\tilde{H}_\varepsilon} e^{-\beta(-\kappa)\varepsilon\mathcal{N}} u_\varepsilon \rangle \le \langle u_\varepsilon, e^{-\beta(-\kappa)\varepsilon\mathcal{N}} u_\varepsilon \rangle. \tag{3.2}$$

The right-hand side can be computed directly from (1.15) and yields

$$\begin{aligned}
\big\langle u_\varepsilon, e^{-\beta(-\kappa)\varepsilon\mathcal{N}} u_\varepsilon \big\rangle &= e^{-\frac{\|u\|^2}{\varepsilon}} \big\langle e^{\frac{a^*(u)}{\sqrt{\varepsilon}}}\Omega, e^{-\beta(-\kappa)\varepsilon\mathcal{N}} e^{\frac{a^*(u)}{\sqrt{\varepsilon}}}\Omega \big\rangle \\
&= e^{-\frac{\|u\|^2}{\varepsilon}} \sum_{k\ge 0}\sum_{\ell\ge 0} \frac{1}{\ell!k!}\frac{1}{\varepsilon^{k/2}\varepsilon^{\ell/2}} \big\langle a^*(u)^\ell\Omega, e^{-\beta(-\kappa)\varepsilon\mathcal{N}} a^*(u)^k\Omega \big\rangle \\
&= e^{-\frac{\|u\|^2}{\varepsilon}} \sum_{\ell\ge 0} \frac{1}{(\ell!)^2}\frac{1}{\varepsilon^\ell} e^{-\varepsilon\beta(-\kappa)\ell} \underbrace{\big\| a^*(u)^\ell\Omega \big\|^2}_{=\ell!\|u\|^{2\ell}} \\
&= e^{-\frac{\|u\|^2}{\varepsilon}} \sum_{\ell\ge 0} \frac{1}{\ell!}\Big(e^{-\varepsilon\beta(-\kappa)} \frac{\|u\|^2}{\varepsilon}\Big)^\ell \\
&= e^{-\|u\|^2(\frac{1-e^{-\beta(-\kappa)\varepsilon}}{\varepsilon})}.
\end{aligned}$$

This directly implies (3.1). ∎

With the exponential decay from Lemma 3.1 we will be able to absorb any polynomial growth in $\|u\|$ that comes from the following estimates.

Lemma 3.2. *For all $m, n \in \mathbb{N}_0$, $s \in [0,1]$, $f \in \ell^2(G)$, and $\varepsilon > 0$ small enough, there exist $C, q > 0$ such that for all $u \in \ell^2(G)$,*

$$\|A_\varepsilon(u)^m e^{is\sqrt{\varepsilon}\Phi(f)}\Phi(f)^n\Omega\| \le C\varepsilon^{m/2}\,\langle\|u\|\rangle^q,$$

where $\langle x\rangle := (1+|x|^2)^{1/2}$ refers to the Japanese bracket. In particular, $q = 0$ for $m = 0$.

Proof. Let $\mathcal{S} = \mathcal{N} + 2$. Then we have

$$
\begin{aligned}
&\left\| A_\varepsilon(u)^m e^{is\sqrt{\varepsilon}\Phi(f)} \Phi(f)^n \Omega \right\| \\
&= \left\| A_\varepsilon(u) \mathcal{S}^{-2} \mathcal{S}^{2} A_\varepsilon(u) \mathcal{S}^{-4} \mathcal{S}^{4} \cdots A_\varepsilon(u) \mathcal{S}^{-2m} \right. \\
&\qquad \left. \times \mathcal{S}^{2m} \Phi(f) \mathcal{S}^{-(2m+1/2)} \mathcal{S}^{2m+1/2} \cdots \Phi(f) \mathcal{S}^{-(2m+n/2)} \mathcal{S}^{2m+n/2} e^{is\sqrt{\varepsilon}\Phi(f)} \Omega \right\| \\
&\leq \prod_{k=1}^{m} \left\| \mathcal{S}^{2k-2} A_\varepsilon(u) \mathcal{S}^{-2k} \right\| \prod_{\ell=1}^{n} \left\| \mathcal{S}^{2m+\ell/2-1/2} \Phi(f) \mathcal{S}^{-(2m+\ell/2)} \right\| \left\| \mathcal{S}^{2m+n/2} e^{is\sqrt{\varepsilon}\Phi(f)} \Omega \right\|.
\end{aligned}
\tag{3.3}
$$

Before estimating each term in the above expression, note that for any function $F : \mathbb{N} \to \mathbb{R}$ and for any $f \in \ell^2(G)$ we have

$$
F(\mathcal{N}) a^*(f) = a^*(f) F(\mathcal{N}+1), \quad F(\mathcal{N}+1) a(f) = a(f) F(\mathcal{N}). \tag{3.4}
$$

Also recall the standard estimates

$$
\left\| a(f)\phi \right\| \leq \|f\| \left\| (\mathcal{N}+1)^{1/2} \phi \right\|, \quad \left\| a^*(f)\phi \right\| \leq \|f\| \left\| (\mathcal{N}+1)^{1/2} \phi \right\| \tag{3.5}
$$

for any $\phi \in D(\mathcal{N}^{1/2})$ and $f \in \ell^2(G)$. We start with the first product in (3.3). Recalling the definition of $A_\varepsilon(u)$ in (2.2) and (2.3) we note that

$$
\begin{aligned}
&\left\| \mathcal{S}^{2k-2} A_\varepsilon(u) \mathcal{S}^{-2k} \right\| \\
&\leq \varepsilon^{1/2} \left\| \mathcal{S}^{2k-2} \left[a\big(h^{\mathrm{H}}(u)\big) + a^*\big(h^{\mathrm{H}}(u)\big) \right] \mathcal{S}^{-2k} \right\| && \text{(3.6a)} \\
&\quad + \varepsilon \left\| \mathcal{S}^{2k-2} \left[d\Gamma(-\Delta_d) - \kappa \mathcal{N} + \frac{\lambda}{2} \sum_{x \in V} \left(a_x^* a_x^* u_x^2 + 4 a_x^* a_x |u_x|^2 + a_x a_x \bar{u}_x^2 \right) \right] \mathcal{S}^{-2k} \right\| && \text{(3.6b)} \\
&\quad + \varepsilon^{3/2} \left\| \mathcal{S}^{2k-2} \left[\frac{\lambda}{2} \sum_{x \in V} (a_x^* a_x^* a_x u_x + a_x^* a_x a_x \bar{u}_x) \right] \mathcal{S}^{-2k} \right\| && \text{(3.6c)} \\
&\quad + \varepsilon^2 \left\| \mathcal{S}^{2k-2} \left[\frac{\lambda}{2} \sum_{x \in V} a_x^* a_x^* a_x a_x \right] \mathcal{S}^{-2k} \right\|. && \text{(3.6d)}
\end{aligned}
$$

Let us deal with each term separately. Using (3.4) and (3.5) we find

$$
\begin{aligned}
\varepsilon^{-1/2} \text{(3.6a)} &\leq \left\| a\big(h^{\mathrm{H}}(u)\big) (\mathcal{N}+1)^{2k-2} (\mathcal{N}+2)^{-2k} \right\| \\
&\quad + \left\| a^*\big(h^{\mathrm{H}}(u)\big) (\mathcal{N}+3)^{2k-2} (\mathcal{N}+2)^{-2k} \right\| \\
&\leq C \left(\left\| a\big(h^{\mathrm{H}}(u)\big) (\mathcal{N}+1)^{-2} \right\| + \left\| a^*\big(h^{\mathrm{H}}(u)\big) (\mathcal{N}+1)^{-2} \right\| \right) \\
&\leq C \left\| h^{H}(u) \right\| \\
&\leq C \left(\|u\| + \|u\|^3 \right).
\end{aligned}
$$

Similarly we have

$$\begin{aligned}\varepsilon^{-1}(3.6b) &\le \left\| d\Gamma(-\Delta_d)\mathcal{S}^{-2}\right\| + \kappa\left\|\mathcal{N}\mathcal{S}^{-2}\right\| \\ &\quad + \frac{\lambda}{2}\sum_{x\in V}|u_x|^2 \left\|a_x^* a_x^*(\mathcal{N}+4)^{2k-2}(\mathcal{N}+2)^{-2k}\right\| \\ &\quad + \frac{\lambda}{2}\sum_{x\in V}4|u_x|^2\left\|a_x^* a_x \mathcal{S}^{-2}\right\| + \frac{\lambda}{2}\sum_{x\in V}|u_x|^2\left\|a_x a_x \mathcal{N}^{2k-2}(\mathcal{N}+2)^{-2k}\right\| \\ &\le C\big(1+\|u\|^2\big),\end{aligned}$$

as well as

$$\begin{aligned}\varepsilon^{-3/2}(3.6c) &\le \frac{\lambda}{2}\sum_{x\in V}|u_x|\left\|a_x^* a_x^* a_x(\mathcal{N}+3)^{2k-2}(\mathcal{N}+2)^{-2k}\right\| \\ &\quad + \frac{\lambda}{2}\sum_{x\in V}|u_x|\left\|a_x^* a_x a_x(\mathcal{N}+1)^{2k-2}(\mathcal{N}+2)^{-2k}\right\| \\ &\le C\big(1+\|u\|\big),\end{aligned}$$

and

$$\varepsilon^{-2}(3.6d) \le \frac{\lambda}{2}\sum_{x\in V}\left\|a_x^* a_x^* a_x a_x(N+2)^{2k-2}(\mathcal{N}+2)^{-2k}\right\| \le C.$$

This implies that

$$\left\|\mathcal{S}^{2k-2}A_\varepsilon(u)\mathcal{S}^{-2k}\right\| \le C\varepsilon^{1/2}\big(1+\|u\|^3\big).$$

Using the same arguments we find

$$\begin{aligned}\left\|\mathcal{S}^{2m+\ell/2-1/2}\Phi(f)\mathcal{S}^{-2m-\ell/2}\right\| &= \left\|\mathcal{S}^{2m+\ell/2-1/2}\frac{1}{\sqrt{2}}\big[a(f)+a^*(f)\big]\mathcal{S}^{-2m-\ell/2}\right\| \\ &\le C\|f\|.\end{aligned}$$

Combining all estimates into (3.3) and noting that

$$e^{-is\sqrt{\varepsilon}\Phi(f)}\mathcal{N}e^{is\sqrt{\varepsilon}\Phi(f)} \le 2\mathcal{N}+1+s^2\varepsilon\|f\|^2,$$

we find

$$\begin{aligned}\left\|A_\varepsilon(u)^m e^{is\sqrt{\varepsilon}\Phi(f)}\Phi(f)^n\Omega\right\| &\le C\bigg(\prod_{k=1}^{m}\varepsilon^{1/2}\big(1+\|u\|^3\big)\bigg)\bigg(\prod_{\ell=1}^{n}\|f\|\bigg) \\ &\le C\varepsilon^{m/2}\langle\|u\|\rangle^q\end{aligned}$$

for $q = 3m/2$, and where the constant C depends on m, n, $\|f\|$, κ, and λ. ∎

3.2. Remainder estimates

In this subsection we first provide an estimate for the remainder term $R_\varepsilon^{(N)}(u, f)$ from Lemma 2.2. Afterwards, we show that the estimate is good enough such that the full remainder in the expansion of the Gibbs state, namely

$$\widetilde{R}_\varepsilon^{(N)}(f) = \int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle} R_\varepsilon^{(N)}(u, f)\, e^{-\beta h(u)} \mathrm{d}u, \tag{3.7}$$

is bounded and of order $\varepsilon^{\frac{N+1}{2}}$.

Lemma 3.3 (Control of the remainder). *There is α with $0 < \alpha < -\kappa$ such that $R_\varepsilon^{(N)}(u, f)$ from Lemma 2.2 satisfies the bound*

$$\left|R_\varepsilon^{(N)}(u, f)\right| \le \varepsilon^{\frac{N+1}{2}} C\langle\|u\|\rangle^q \left(1 + e^{\beta(h(u)-\alpha\|u\|^2)}\right) \tag{3.8}$$

for all $\varepsilon > 0$ small enough, where C depends on N, κ, λ, β and f.

Proof. By Lemma 2.2, the expression $R_\varepsilon^{(N)}(u, f)$ is composed of four terms which we estimate separately. We assume $\varepsilon \le 1$ in the following estimates. Using first some elementary bounds and Cauchy–Schwarz, then Lemma 3.2 for $s = 0$, then

$$\widetilde{W}_\varepsilon(u)^* H_\varepsilon \widetilde{W}_\varepsilon(u) = h(u) + A_\varepsilon(u),$$

and in the end Lemma 3.1, we find

$$\begin{aligned}
&\left|\langle\Omega, \mathcal{R}_A^{(N)}\mathcal{M}_f^{(N)}\Omega\rangle\right| \\
&= \left|\frac{(-\beta)^{N+1}}{N!}\sum_{n=0}^{N} \varepsilon^{\frac{n}{2}}\frac{i^n}{n!}\int_0^1 (1-s)^N\langle\Omega, A_\varepsilon(u)^{N+1}e^{-s\beta A_\varepsilon(u)}\Phi(f)^n\,\Omega\rangle \mathrm{d}s\right| \\
&\le \frac{\beta^{N+1}}{N!}\sum_{n=0}^{N}\frac{1}{n!}\int_0^1 \left|\langle\Omega, A_\varepsilon(u)^{N+1}e^{-s\beta A_\varepsilon(u)}\Phi(f)^n\,\Omega\rangle\right|\mathrm{d}s \\
&\le \frac{\beta^{N+1}}{N!}\sum_{n=0}^{N}\frac{1}{n!}\int_0^1 \|e^{-s\beta A_\varepsilon(u)}\Omega\|\left\|A_\varepsilon(u)^{N+1}\Phi(f)^n\,\Omega\right\|\mathrm{d}s \\
&\le \varepsilon^{\frac{N+1}{2}} C\langle\|u\|\rangle^q \int_0^1 \sqrt{\langle\Omega, e^{-2s\beta A_\varepsilon(u)}\Omega\rangle}\mathrm{d}s \\
&= \varepsilon^{\frac{N+1}{2}} C\langle\|u\|\rangle^q \int_0^1 e^{s\beta h(u)}\sqrt{\langle u_\varepsilon, e^{-2s\beta H_\varepsilon}u_\varepsilon\rangle}\mathrm{d}s \\
&\le \varepsilon^{\frac{N+1}{2}} C\langle\|u\|\rangle^q \int_0^1 e^{s\beta h(u)}e^{-s\beta\alpha\|u\|^2}\mathrm{d}s.
\end{aligned}$$

The other terms can be estimated similarly, using again Lemmas 3.1 and 3.2. We have

$$\begin{aligned}
&\left|\left\langle \Omega, \mathcal{R}_A^{(N)} \mathcal{R}_f^{(N)} \Omega \right\rangle\right| \\
&= \left| \varepsilon^{\frac{N+1}{2}} \frac{(-\beta)^{N+1}}{N!} \frac{i^{N+1}}{N!} \int_0^1 \mathrm{d}\tilde{s}\,(1-\tilde{s})^N \right. \\
&\qquad \left. \times \int_0^1 \mathrm{d}s\,(1-s)^N \left\langle \Omega, A_\varepsilon(u)^{N+1} e^{-s\beta A_\varepsilon(u)} e^{i\tilde{s}\sqrt{\varepsilon}\Phi(f)} \Phi(f)^{N+1}\,\Omega \right\rangle \right| \\
&\le \varepsilon^{\frac{N+1}{2}} \frac{\beta^{N+1}}{N!} \frac{1}{N!} \int_0^1 \mathrm{d}\tilde{s} \int_0^1 \mathrm{d}s \left\| e^{-s\beta A_\varepsilon(u)} \Omega \right\| \left\| A_\varepsilon(u)^{N+1} e^{i\tilde{s}\sqrt{\varepsilon}\Phi(f)} \Phi(f)^{N+1} \Omega \right\| \\
&\le \varepsilon^{N+1} C \langle \|u\| \rangle^q \int_0^1 e^{s\beta h(u)} e^{-s\beta\alpha\|u\|^2} \mathrm{d}s,
\end{aligned}$$

as well as

$$\begin{aligned}
&\left|\left\langle \Omega, \mathcal{M}_A^{(N)} \mathcal{R}_f^{(N)} \Omega \right\rangle\right| \\
&= \left| \varepsilon^{\frac{N+1}{2}} \frac{i^{N+1}}{N!} \sum_{m=0}^{N} \frac{(-\beta)^m}{m!} \int_0^1 (1-s)^N \left\langle \Omega, A_\varepsilon(u)^m e^{is\sqrt{\varepsilon}\Phi(f)} \Phi(f)^{N+1} \Omega \right\rangle \mathrm{d}s \right| \\
&\le \varepsilon^{\frac{N+1}{2}} \frac{1}{N!} \sum_{m=0}^{N} \frac{\beta^m}{m!} \left\| A_\varepsilon(u)^m \Omega \right\| \left\| \Phi(f)^{N+1} \Omega \right\| \\
&\le \varepsilon^{\frac{N+1}{2}} C \langle \|u\| \rangle^q .
\end{aligned}$$

Lastly,

$$\begin{aligned}
&\left|\left\langle \Omega, \mathcal{R}_{f,A}^{(N)} \Omega \right\rangle\right| \\
&= \left| \sum_{j=N+1}^{5N-2} \varepsilon^{\frac{j}{2}} \sum_{m=1}^{j} \frac{(-\beta)^m}{m!} \sum_{\ell=\max(m,j-N)}^{\min(4m-2,j)} \frac{i^{j-\ell}}{(j-\ell)!} \left\langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{j-\ell}\,\Omega \right\rangle \right| \\
&\le \sum_{j=N+1}^{5N-2} \varepsilon^{\frac{j}{2}} \sum_{m=1}^{j} \frac{\beta^m}{m!} \sum_{\ell=\max(m,j-N)}^{\min(4m-2,j)} \frac{1}{(j-\ell)!} \left\| A_\ell^{(m)}(u)\Omega \right\| \left\| \Phi(f)^{j-\ell}\,\Omega \right\| \\
&\le \varepsilon^{\frac{N+1}{2}} C \langle \|u\| \rangle^q ,
\end{aligned}$$

since $\|A_\ell^{(m)}(u)\Omega\| \le C\langle \|u\| \rangle^q$ by repeatedly applying the standard estimates (3.5). To conclude the bound (3.8) recall that α from Lemma 3.1 satisfies $0 < \alpha < -\kappa$, and that $h(u) \ge -\kappa\|u\|^2$ (with $\kappa < 0$), hence $h(u) - \alpha\|u\|^2 > 0$ and

$$\int_0^1 e^{s\beta(h(u)-\alpha\|u\|^2)} \mathrm{d}s \le e^{\beta(h(u)-\alpha\|u\|^2)}. \qquad \blacksquare$$

From Lemma 3.3 we know that the full remainder $\widetilde{R}_\varepsilon^{(N)}(f)$ from (3.7) is of order $\varepsilon^{\frac{N+1}{2}}$. It remains to prove the integrability in u.

Lemma 3.4 (Integrability of the remainder). *For all $N \in \mathbb{N}$ we have*

$$\left|\widetilde{R}_\varepsilon^{(N)}(f)\right| \le C\varepsilon^{\frac{N+1}{2}}.$$

Proof. Applying Lemma 3.3 leads to

$$\begin{aligned}
&\left|\int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle} R_\varepsilon^{(N)}(u,f)e^{-\beta h(u)}\mathrm{d}u\right| \\
&\quad\le C\varepsilon^{\frac{N+1}{2}}\int_{\ell^2(G)} \langle\|u\|\rangle^q \left(1+e^{\beta h(u)-\beta\alpha\|u\|^2}\right)e^{-\beta h(u)}\mathrm{d}u \\
&\quad\le C\varepsilon^{\frac{N+1}{2}}\int_{\ell^2(G)} \langle\|u\|\rangle^q \left(e^{-\beta h(u)}+e^{-\beta\alpha\|u\|^2}\right)\mathrm{d}u \\
&\quad\le C\varepsilon^{\frac{N+1}{2}}
\end{aligned}$$

since $\beta > 0$ and $\alpha > 0$. ■

We can now put everything together to prove our main theorem.

Proof of Theorem 1.1. Combining Lemmas 2.1 and 2.2 we find, for any $M \in \mathbb{N}$,

$$(\varepsilon\pi)^{|V|}\operatorname{Tr}\left(e^{-\beta H_\varepsilon}W(f)\right) - \sum_{j=0}^{M}\varepsilon^{\frac{j}{2}}\int_{\ell^2(G)} e^{\sqrt{2}i\Re e\langle f,u\rangle}C_{\frac{j}{2}}(u,f)e^{-\beta h(u)}\mathrm{d}u = \widetilde{R}_\varepsilon^{(M)}(f),$$

where the first summand in the definition of $C_{\frac{j}{2}}(u,f)$ from (2.11) is given by Lemma 2.4, and with remainder $\widetilde{R}_\varepsilon^{(M)}(f)$ defined in (3.7). In Lemma 3.4 we have proved that

$$\left|\widetilde{R}_\varepsilon^{(M)}(f)\right| \le C\varepsilon^{\frac{M+1}{2}}.$$

All coefficients $C_{\frac{j}{2}}(u,f)$ with odd j vanish by Lemma 2.3. Thus, for $M =: 2N+1$ odd we have

$$\left|\widetilde{R}_\varepsilon^{(2N+1)}(f)\right| \le C\varepsilon^{N+1},$$

and for $M =: 2N+2$ even we have $|\widetilde{R}_\varepsilon^{(2N+1)}(f)| \le C\varepsilon^{N+\frac{3}{2}} \le C\varepsilon^{N+1}$ as well. ■

Appendix: Computation of the first two coefficients

Here, we compute the coefficients $C_1(u,f)$ and $C_2(u,f)$ from Theorem 1.1 explicitly. Recall that

$$\begin{aligned}
C_j(u,f) &= \frac{(-1)^j}{j!\,4^j}\|f\|^{2j} \\
&\quad+ \sum_{m=1}^{2j}\frac{(-\beta)^m}{m!}\sum_{\ell=m}^{\min(4m-2,2j)}\frac{i^{2j-\ell}}{(2j-\ell)!}\left\langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{2j-\ell}\,\Omega\right\rangle.
\end{aligned}$$

We then find

$$
\begin{aligned}
C_1(u,f) &= -\frac{1}{4}\|f\|^2 - \beta\sum_{\ell=1}^{2}\frac{i^{2-\ell}}{(2-\ell)!}\big\langle A_\ell^{(1)}(u)\Omega, \Phi(f)^{2-\ell}\,\Omega\big\rangle + \frac{\beta^2}{2!}\big\langle A_2^{(2)}(u)\Omega,\Omega\big\rangle \\
&= -\frac{1}{4}\|f\|^2 - \beta i\big\langle A_1^{(1)}(u)\Omega, \Phi(f)\Omega\big\rangle - \beta\big\langle A_2^{(1)}(u)\Omega,\Omega\big\rangle + \frac{\beta^2}{2!}\big\langle A_2^{(2)}(u)\Omega,\Omega\big\rangle,
\end{aligned}
$$

where, by the definition (2.8), $A_1^{(1)} = A_1$, $A_2^{(1)} = A_2$, and $A_2^{(2)} = A_1A_1$. Now, recalling the definition (2.3) and using that $a(g)\Omega = 0$ for any $g \in \ell^2(G)$, we have

$$
\begin{aligned}
&\big\langle A_1^{(1)}(u)\Omega, \Phi(f)\Omega\big\rangle = \frac{1}{\sqrt{2}}\big\langle a^*\big(h^{\mathrm{H}}(u)\big)\Omega, a^*(f)\Omega\big\rangle = \frac{1}{\sqrt{2}}\big\langle h^{\mathrm{H}}(u), f\big\rangle, \\
&\big\langle A_2^{(1)}(u)\Omega,\Omega\big\rangle = 0, \\
&\big\langle A_2^{(2)}(u)\Omega,\Omega\big\rangle = \big\langle a^*\big(h^{\mathrm{H}}(u)\big)\Omega, a^*\big(h^{\mathrm{H}}(u)\big)\Omega\big\rangle = \big\|h^{\mathrm{H}}(u)\big\|^2.
\end{aligned}
$$

To summarize,

$$
C_1(u,f) = -\frac{\|f\|^2}{4} - i\frac{\beta}{\sqrt{2}}\langle h^{\mathrm{H}}(u), f\rangle + \frac{\beta^2}{2}\|h^{\mathrm{H}}(u)\|^2.
$$

The second coefficient is given by

$$
\begin{aligned}
&C_2(u,f) \\
&= \frac{1}{32}\|f\|^4 + \sum_{m=1}^{4}\frac{(-\beta)^m}{m!}\sum_{\ell=m}^{\min(4m-2,4)}\frac{i^{4-\ell}}{(4-\ell)!}\big\langle A_\ell^{(m)}(u)\Omega, \Phi(f)^{4-\ell}\,\Omega\big\rangle \\
&= \frac{1}{32}\|f\|^4 - \beta\Big(-\frac{i}{6}\big\langle A_1^{(1)}(u)\Omega, \Phi(f)^3\Omega\big\rangle - \frac{1}{2}\big\langle A_2^{(1)}(u)\Omega, \Phi(f)^2\,\Omega\big\rangle\Big) \\
&\quad + \frac{\beta^2}{2}\Big(-\frac{1}{2}\big\langle A_2^{(2)}(u)\Omega, \Phi(f)^2\,\Omega\big\rangle + i\big\langle A_3^{(2)}(u)\Omega, \Phi(f)\Omega\big\rangle + \big\langle A_4^{(2)}(u)\Omega,\Omega\big\rangle\Big) \\
&\quad - \frac{\beta^3}{6}\big(i\big\langle A_3^{(3)}(u)\Omega, \Phi(f)\Omega\big\rangle + \big\langle A_4^{(3)}(u)\Omega,\Omega\big\rangle\big) + \frac{\beta^4}{24}\big\langle A_4^{(4)}(u)\Omega,\Omega\big\rangle.
\end{aligned}
$$

Using again the definitions (2.3) and (2.8) we find explicitly

$$
\begin{aligned}
&C_2(u,f) \\
&= \frac{1}{32}\|f\|^4 - \beta\Big(-\frac{i}{4\sqrt{2}}\|f\|^2\big\langle h^{\mathrm{H}}(u), f\big\rangle - \frac{\lambda}{8}\langle u^2, f^2\rangle\Big) \\
&\quad + \beta^2\Big(-\frac{1}{8}\big\|h^{\mathrm{H}}(u)\big\|^2\|f\|^2 - \frac{1}{4}\big\langle h^{\mathrm{H}}(u), f\big\rangle^2 + \frac{\lambda i}{2\sqrt{2}}\big\langle u^2, h^{\mathrm{H}}(u)f\big\rangle - \frac{\kappa i}{2\sqrt{2}}\big\langle h^{\mathrm{H}}(u), f\big\rangle \\
&\qquad + \frac{i}{2\sqrt{2}}\big\langle h^{\mathrm{H}}(u), -\Delta_d f\big\rangle + \frac{\lambda i}{\sqrt{2}}\big\langle u h^{\mathrm{H}}(u), uf\big\rangle + \frac{\lambda^2}{4}\sum_{x\in V}|u_x|^4\Big) \\
&\quad - \beta^3\Big(\frac{i}{2\sqrt{2}}\big\langle h^{\mathrm{H}}(u), f\big\rangle\big\|h^{\mathrm{H}}(u)\big\|^2 + \frac{\lambda}{6}\big\langle u^2, h^{\mathrm{H}}(u)^2\big\rangle + \frac{1}{6}\big\langle h^{\mathrm{H}}(u), -\Delta_d h^{\mathrm{H}}(u)\big\rangle \\
&\qquad - \frac{\kappa}{6}\big\|h^{\mathrm{H}}(u)\big\|^2 + \frac{\lambda}{3}\big\|u h^{\mathrm{H}}(u)\big\|^2 + \frac{\lambda}{6}\big\langle h^{\mathrm{H}}(u)^2, u^2\big\rangle\Big) + \frac{\beta^4}{8}\big\|h^{\mathrm{H}}(u)\big\|^4.
\end{aligned}
$$

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Zied Ammari
Institut de recherche mathématique de Rennes - IRMAR, Université de Rennes, Campus de Beaulieu, 263, avenue du Général Leclerc, 35042 Rennes, France; zied.ammari@univ-rennes.fr

Shahnaz Farhat
School of Science, Constructor University Bremen, Campus Ring 1, 28759 Bremen, Germany; sfarhat@constructor.university

Sören Petrat
School of Science, Constructor University Bremen, Campus Ring 1, 28759 Bremen, Germany; spetrat@constructor.university