



Dyson expansion for form-bounded perturbations and applications to the polaron problem

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Received: 8 January 2026 / Revised: 14 May 2026 / Accepted: 15 June 2026
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Abstract

We present an abstract Dyson expansion for perturbations that are merely relatively form-bounded, and apply it to the polaron problem. For a large class of polaron-type models, including the Fröhlich and Nelson models, we prove that the vacuum expectation value of the heat semi-group is a completely monotone function of the square of the total momentum. Consequently, the ground-state energy is a concave function of the square of the momentum, a result recently proved for the Fröhlich model in [14] using a probabilistic approach via Wiener integrals.

Keywords Dyson expansion · Quadratic forms · Polaron · Ground state energy

Mathematics Subject Classification 81V73 · 81Q1 · 46N50

1 Introduction and main results

The polaron problem concerns the interaction of a charged particle with the excitations of a medium modeled by a bosonic field. Examples include the Fröhlich model [5] describing the coupling between an electron and the phonon modes of a polarized crystal, or the Nelson model [13] of quantum electrodynamics. In this paper, we shall consider a general class of polaron Hamiltonians, formally given by

$$\mathbb{H}(P) = |P - \mathbb{P}_f|^2 + d\Gamma(\omega) + \Phi(v) \quad (1.1)$$

for $P \in \mathbb{R}^d$ corresponding to the total momentum of the system. The operators (1.1) act on the bosonic Fock space $\mathfrak{F}_s(L^2(\mathbb{R}^d)) = \mathbb{C} \oplus \bigoplus_{N=1}^{\infty} L_s^2(\mathbb{R}^{dN})$, where $L_s^2(\mathbb{R}^{dN}) \subset$

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$L^2(\mathbb{R}^{dN})$ denotes the subspace of permutation-invariant functions of N (momentum) variables $k_1, \dots, k_N \in \mathbb{R}^d$. Here, the field energy $d\Gamma(\omega) := \int_{\mathbb{R}^d} \omega(k) a_k^* a_k dk$ is the second quantization of a non-negative Fourier multiplier ω , and $\mathbb{P}_f := d\Gamma(k)$ is the field momentum operator. The interaction of the particle with the field modes is described by the field operator $\Phi(v) = a^\dagger(v) + a(v)$, where $a^\dagger(f)$ and $a(f)$ are, for $f \in L^2(\mathbb{R}^d)$, the usual creation and annihilation operators, satisfying the canonical commutation relations $[a(f), a^\dagger(g)] = \langle f|g \rangle$. The Hamiltonians (1.1) result from a restriction of the system to the sector of total momentum P , applying the Lee–Low–Pines transformation [9].

The usual Fröhlich model corresponds to $d = 3$, $\omega \equiv 1$, and $v(k) = \sqrt{\alpha/(2\pi^2)}|k|^{-1}$ for some coupling constant $\alpha > 0$. For the Nelson model, $\omega(k) = |k|$ (or, more generally, $\omega(k) = \sqrt{|k|^2 + m^2}$ for $m \geq 0$) and $v(k)$ is proportional to $|k|^{-1/2}$, which needs to be suitably cut off at large momentum to avoid an ultraviolet divergence, however. In general, the Hamiltonian (1.1) is well-defined as a quadratic form and bounded from below, under the following assumptions on v and ω .

Assumption 1 We assume that $\omega : \mathbb{R}^d \rightarrow \mathbb{R}_+$, and that the interaction v is of the form $v = v_1 + v_2$ with

$$\int_{\mathbb{R}^d} \frac{|v_1(k)|^2}{\omega(k)} dk < \infty \quad \text{and} \quad \int_{\mathbb{R}^d} \frac{|v_2(k)|^2}{|k|^2} \left(1 + \frac{1}{\omega(k)}\right) dk < \infty. \quad (1.2)$$

The first condition in (1.2) can be viewed as a condition on infrared regularity, while the second concerns the ultraviolet behavior of v . Under Assumption 1, the commutator method of Lieb–Yamazaki [10] shows that $\Phi(v)$ is infinitesimally form-bounded with respect to $|P - \mathbb{P}_f|^2 + d\Gamma(\omega)$, and hence, $\mathbb{H}(P)$ defines a semi-bounded self-adjoint operator via its quadratic form [16, Thm. X.17]. For completeness, we shall repeat this argument in Appendix A. If $\omega(k) \equiv 1$, the condition (1.2) becomes $\int_{\mathbb{R}^d} |v(k)|^2 (1 + |k|^2)^{-1} dk < \infty$ and is satisfied for $v(k) = g|k|^{-\beta}$ for $(d-2)/2 < \beta < d/2$ and $g \in \mathbb{C}$, for instance. If $\omega(k) = |k|$, on the other hand, $(d-2)/2 < \beta < (d-1)/2$ would be admissible.

To state our main results, we need to introduce some notation. For $n \geq 1$, let S_{2n} denote the set of permutations of $2n$ elements, and let $\mathcal{W}_{2n} \subset S_{2n}$ be the set of Wick pairings, i.e., those permutations satisfying $\pi(2j-1) < \pi(2j+1)$ for $j \in \{1, \dots, n-1\}$ and $\pi(2j-1) < \pi(2j)$ for $j \in \{1, \dots, n\}$. Permutations in $\mathcal{W}_{2n}$ are in one-to-one correspondence with partitions into sets of cardinality two, i.e., n pairings $(\pi(2i-1), \pi(2i))$, $1 \leq i \leq n$, of the numbers $\{1, \dots, 2n\}$. Moreover, we shall denote by $\mathcal{W}_{2n}^0 \subset \mathcal{W}_{2n}$ those permutations that correspond to pairings that interlace, i.e., cannot be decomposed into pairings within disjoint subintervals; explicitly, $\pi \in \mathcal{W}_{2n}$ is an element of $\mathcal{W}_{2n}^0$ if and only if $\sum_{j=1}^{\ell} (-1)^{\pi^{-1}(j)} < 0$ for all $1 \leq \ell < 2n$.

For $\pi \in \mathcal{W}_{2n}$ and $1 \leq j \leq 2n-1$, let

$$\mathcal{M}_j^\pi = \{1 \leq i \leq n : \pi(2i-1) \leq j < \pi(2i)\} \subset \{1, \dots, n\} \quad (1.3)$$

corresponding to the set of pairs whose connecting line crosses j (which may be empty). For convenience, we shall also introduce $\mathcal{M}_0^\pi = \mathcal{M}_{2n}^\pi = \emptyset$. For

$\underline{k} = (k_1, \dots, k_n) \in \mathbb{R}^{dn}$ and $0 \leq j \leq 2n$, let

$$\mathcal{E}_P^{(\pi, j)}(\underline{k}) = \left| P - \sum_{\ell \in \mathcal{M}_j^\pi} k_\ell \right|^2 + \sum_{\ell \in \mathcal{M}_j^\pi} \omega(k_\ell). \quad (1.4)$$

We shall denote by Δ_k^t the simplex

$$\Delta_k^t = \{(t_0, \dots, t_k) = \underline{t} \in \mathbb{R}_+^{k+1}, \sum_{i=0}^k t_i = t\}. \quad (1.5)$$

Finally, we shall use the notation $\Omega = (1, 0, 0, \dots) \in \mathfrak{F}_s(L^2(\mathbb{R}^d))$ for the vacuum vector.

Our first main result is summarized in the following Theorem.

Theorem 1 *For $\pi \in \mathcal{W}_{2n}$, the set of Wick pairings defined above, let $\mathcal{E}_P^{(\pi, j)}$ be given in (1.4). Under Assumption 1, the following holds:*

(a) *For $t > 0$, we have the convergent expansion*

$$\langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle = e^{-t|P|^2} + \sum_{n \geq 1} \sum_{\pi \in \mathcal{W}_{2n}} \int_{\Delta_{2n}^t} \int_{\mathbb{R}^{dn}} e^{-\sum_{j=0}^{2n} t_j \mathcal{E}_P^{(\pi, j)}(\underline{k})} \prod_{j=1}^n |v(k_j)|^2 dk_j d\underline{t} \quad (1.6)$$

where the outer integral is over the simplex Δ_{2n}^t defined in (1.5).

(b) *For $t > 0$, we further have the renewal equation*

$$\begin{aligned} \langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle &= e^{-t|P|^2} \\ &+ \int_0^t \langle \Omega | e^{-(t-s)\mathbb{H}(P)} \Omega \rangle \sum_{n \geq 1} \sum_{\pi \in \mathcal{W}_{2n}^0} \int_{\Delta_{2n-1}^s} \int_{\mathbb{R}^{dn}} e^{-\sum_{j=0}^{2n-1} t_j \mathcal{E}_P^{(\pi, j)}(\underline{k})} \prod_{j=1}^n |v(k_j)|^2 dk_j d\underline{t} ds \end{aligned} \quad (1.7)$$

where $\mathcal{W}_{2n}^0 \subset \mathcal{W}_{2n}$ are the interlacing Wick pairings defined above.

The identity (1.6) formally follows from a Dyson expansion of $e^{-t\mathbb{H}(P)}$ in terms of the interaction $\Phi(v)$, but it is a priori not clear how to make sense of such an expansion in the low-regularity setting considered here, where $\Phi(v)$ is unbounded and merely form-bounded relative to the non-interacting Hamiltonian. An abstract result applicable to this setting will be presented in Sect. 2 and will be the starting point in the proof of Theorem 1. Part (b) of the theorem is inspired by [14], where a renewal equation for $\langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle$ was derived in the Fröhlich case, using a closely related probabilistic approach via Wiener integrals.

Theorem 1 turns out to be very useful in studying the momentum dependence $P \mapsto \langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle$ for fixed $t > 0$. We shall need the following additional assumption on v and ω . Recall that, according to Bernstein's theorem [4], a function on $\mathbb{R}_+$ is completely monotone if and only if it is the Laplace transform of a positive measure.

Assumption 2 Assume that ω and v are radial, and that the function

$$|P|^2 \mapsto \int_{\mathbb{R}^d} |v(k)|^2 e^{-r|P-k|^2 - s\omega(k)} dk \quad (1.8)$$

is completely monotone for any $r > 0$ and $s > 0$.

For $\omega \equiv 1$, this additional assumption is fulfilled for $v(k) = g|k|^{-\beta}$ for any $\beta \geq 0$, as one can see by writing $|v(k)|^2$ as an integral over Gaussians,

$$\Gamma(\beta)|k|^{-2\beta} = \int_0^\infty e^{-|k|^2 x} x^{\beta-1} dx \quad (1.9)$$

for $\beta > 0$, and noting that the convolution of two Gaussians is again a Gaussian. The same applies to $\omega(k) = \sqrt{|k|^2 + m^2}$ for $m \geq 0$, since in this case also $e^{-s\omega(k)}$ can be written as an average over Gaussians:

$$e^{-s\sqrt{|k|^2 + m^2}} = \int_0^\infty \frac{e^{-x}}{\sqrt{\pi x}} e^{-\frac{x^2}{4x}(|k|^2 + m^2)} dx. \quad (1.10)$$

The assumption is thus satisfied for both the Fröhlich and the Nelson models, if in the latter case, the ultraviolet cutoff is chosen in a suitable way to respect the complete positivity of (1.8), e.g., via a Gaussian factor as $v(k) = g|k|^{-1/2}e^{-\varepsilon|k|^2}$ for $\varepsilon > 0$. Since the cutoff can be removed, i.e., the limit $\varepsilon \rightarrow 0$ taken, after the subtraction of a diverging (but P -independent) constant, the following consequently also holds for the renormalized Nelson model.

Corollary 1 Under Assumptions 1 and 2, the following holds:

- (a) $|P|^2 \mapsto \langle \Omega | e^{-t\mathbb{H}(P)} | \Omega \rangle$ is completely monotone for any $t > 0$.
- (b) If $v \not\equiv 0$, then $|P|^2 \mapsto E_0(P) = \inf \text{spec } \mathbb{H}(P)$ is concave, and in fact strictly concave on the set of P s where $\mathbb{H}(P)$ has a ground state.

The existence of a ground state of $\mathbb{H}(P)$ is guaranteed if $E_0(P) < E_{\text{ess}}(P)$, where $E_{\text{ess}}(P)$ denotes the bottom of the essential spectrum of $\mathbb{H}(P)$. Under additional regularity assumptions on ω , it is known to have the explicit form [12]

$$E_{\text{ess}}(P) = \inf_{n \geq 1} \inf_{k_1, \dots, k_n} \left\{ E_0 \left(P - \sum_{j=1}^n k_j \right) + \sum_{j=1}^n \omega(k_j) \right\}. \quad (1.11)$$

In the case of the Fröhlich model, the infimum is attained at $n = 1$ and $k_1 = P$, hence $E_{\text{ess}}(P) = E_0(0) + 1$ for any $P \in \mathbb{R}^d$.

Since a completely monotone function is log-convex, the concavity in (b) follows immediately from (a), using that

$$E_0(P) = - \lim_{t \rightarrow \infty} \frac{1}{t} \ln \langle \Omega | e^{-t\mathbb{H}(P)} | \Omega \rangle. \quad (1.12)$$

If $v \equiv 0$, (1.12) holds only whenever $E_0(P) < E_{\text{ess}}(P)$, but if $v \not\equiv 0$, it actually holds for any $P \in \mathbb{R}^d$, by a Perron–Frobenius type argument [7, 8, 11] (see also [6])

and references there). To obtain strict concavity, the renewal equation of part (b) in Theorem 1 will be useful, similarly as in [14].

The concavity of $|P|^2 \mapsto E_0(P)$ has played an important role in the recent proof of the validity of the Landau–Pekar formula for the effective mass of the Fröhlich model in the strong coupling limit, see [2, 3].

2 Abstract Dyson expansion for form-bounded perturbations

Let $A \geq 0$ be a self-adjoint operator. Let B be a symmetric quadratic form that is form-bounded with respect to A with relative bound less than 1, i.e., there exist $a \geq 0$ and $0 < \lambda < 1$ such that

$$|B(\psi, \psi)| \leq \lambda \left(\|\sqrt{A}\psi\| + a\|\psi\|^2 \right) \quad (2.1)$$

for any ψ in the quadratic form domain of A (i.e., the domain of $\sqrt{A}$). Then, the semi-bounded quadratic form $\|\sqrt{A}\psi\|^2 + B(\psi, \psi)$ (defined on the form domain of A) defines a unique self-adjoint operator [16, Thm. X.17], which we shall denote by $A + B$. Let

$$C = (A + a)^{-1/2}(A + B)(A + a)^{-1/2} - A(A + a)^{-1} \quad (2.2)$$

which one readily checks to be a bounded operator satisfying $\|C\| \leq \lambda < 1$. It will be convenient to think of B as formally given by $B = \sqrt{A + a}C\sqrt{A + a}$; the precise way to interpret this identity is $A + B + a = \sqrt{A + a}(C + 1)\sqrt{A + a}$, which directly follows from the definitions.

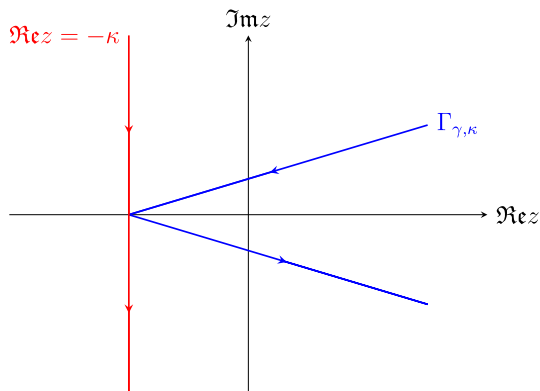
Our goal in this section is to justify the Dyson expansion, formally given by

$$e^{-t(A+B)} = e^{-tA} + \sum_{n \geq 1} (-1)^n \int_{\Delta_n^t} e^{-t_0 A} B e^{-t_1 A} \dots B e^{-t_n A} dt \quad (2.3)$$

for $t > 0$, where the integral is over the simplex Δ_n^t defined in (1.5). However, in the general setting considered here, where B is merely form-bounded relative to A , it is not clear how to even make sense of the integrals on the right-hand side. Note that even under the stronger assumption that B is operator-bounded relative to A , the validity of (2.3) is not known, in general; we refer to [1, 15] for partial results in this direction.

The following theorem states that under the assumption (2.1) above, $e^{-t(A+B)}$ indeed has a convergent expansion in powers of B , but the individual terms in the expansion cannot necessarily be written in the form (2.3). This will be sufficient for our application in the proof of Theorem 1, however.

Theorem 2 *Let $A \geq 0$ be a self-adjoint operator, B a relatively form-bounded perturbation satisfying (2.1) for $0 \leq \lambda < 1$ and $a \geq 0$, and let $A + B$ be defined as above.*

Fig. 1 The contour $\Gamma_{\gamma,\kappa}$ 

Then, for $t > 0$, there exist bounded operators D_n satisfying

$$\|D_n\| \leq \frac{e^{3/2}}{\pi} \sqrt{n+2} \lambda^n e^{ta} \quad (2.4)$$

such that one has the norm-convergent expansion

$$e^{-t(A+B)} = e^{-tA} + \sum_{n \geq 1} D_n \quad (2.5)$$

The proof gives an explicit formula for D_n in terms of a contour integral and the operator C in (2.2), see Eq. (2.12). For bounded B , one can show that it agrees with the n 'th term on the right-hand side of (2.3).

Proof By absorbing a into A , we can set $a = 0$ without loss of generality, and assume that A has a bounded inverse. We start with the contour integral representation

$$e^{-t(A+B)} = \frac{1}{2\pi i} \int_{\Gamma_{\gamma,\kappa}} e^{-tz} \frac{1}{z - A - B} dz \quad (2.6)$$

for the contour

$$\Gamma_{\gamma,\kappa} = \{z \in \mathbb{C} : \Re z = -\kappa + \gamma|\Im z|\} \quad (2.7)$$

for some $\gamma > 0$ and $\kappa > 0$, integrated counter-clockwise (i.e., from top to bottom), see Fig. 1.

In the following, we shall use that the distance between $\Gamma_{\gamma,\kappa}$ and a point on the positive real axis is

$$\inf_{z \in \Gamma_{\gamma,\kappa}} |z - \lambda| = \frac{\kappa + \lambda}{(1 + \gamma^2)^{1/2}} \quad \text{for } \lambda > 0. \quad (2.8)$$

With C defined as in (2.2) (with $a = 0$), we have the identity

$$z - A - B = \sqrt{A} \left(1 - CA(z - A)^{-1}\right) A^{-1/2} (z - A). \quad (2.9)$$

Moreover, for $z \in \Gamma_{\gamma, \kappa}$, (2.8) implies that

$$\|A(z - A)^{-1}\| \leq \sup_{\lambda > 0} \frac{\lambda}{|z - \lambda|} \leq (1 + \gamma^2)^{1/2} \quad (2.10)$$

and hence $\|CA(z - A)^{-1}\| < 1$ for γ small enough. Under this assumption on γ , we thus have the convergent Neumann series

$$\begin{aligned} (z - A - B)^{-1} &= A^{1/2}(z - A)^{-1} \left(1 - CA(z - A)^{-1}\right)^{-1} A^{-1/2} \\ &= \frac{A^{1/2}}{z - A} \sum_{n \geq 0} \left(C \frac{A}{z - A}\right)^n A^{-1/2}. \end{aligned} \quad (2.11)$$

By dominated convergence, we can interchange the sum and the integral. In particular, we conclude that (2.5) holds with

$$D_n = \frac{1}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} e^{-tz} \frac{A^{1/2}}{z - A} \left(C \frac{A}{z - A}\right)^{n-1} C \frac{A^{1/2}}{z - A} dz \quad (2.12)$$

for $n \geq 1$. Note that D_n is actually independent of γ and κ . Since

$$\|A^{1/2}(z - A)^{-1}\| \leq \sup_{\lambda > 0} \frac{\sqrt{\lambda}}{|z - \lambda|} \leq (1 + \gamma^2)^{1/2} \kappa^{-1/2} \quad (2.13)$$

for $z \in \Gamma_{\gamma, \kappa}$ (again using (2.8)), the norm of D_n is bounded as

$$\|D_n\| \leq \frac{1}{2\pi \kappa} (1 + \gamma^2)^{(n+1)/2} \|C\|^n \int_{\Gamma_{\gamma, \kappa}} e^{-t\Re z} |dz| = \frac{e^{t\kappa}}{\pi \kappa \gamma t} (1 + \gamma^2)^{n/2+1} \|C\|^n. \quad (2.14)$$

The optimal choice of κ and γ is thus $\kappa = 1/t$, $\gamma^2 = (n+1)^{-1}$, leading to

$$\|D_n\| \leq \frac{e}{\pi} \frac{(n+2)^{(n+2)/2}}{(n+1)^{(n+1)/2}} \|C\|^n \leq \frac{e^{3/2}}{\pi} \sqrt{n+2} \|C\|^n \quad (2.15)$$

uniformly in $t > 0$, and thus to the claim in (2.4) after shifting back by a . $\square$

Remark 1 The proof above can be modified to also show that

$$\|\sqrt{A}D_n\sqrt{A}\| \leq \frac{e}{\pi t} \frac{(n+2)^{(n+2)/2}}{(n+1)^{(n+1)/2}} \|C\|^n \quad (2.16)$$

which diverges as $t \rightarrow 0$, however.

3 Application to the polaron model

We shall now apply the result of the previous section to the polaron problem. We shall write $\mathbb{H}(P) = A + B - a$ for suitable (i.e., large enough) $a \geq 0$, with

$$A = |P - \mathbb{P}_f|^2 + d\Gamma(\omega) + a \quad (3.1)$$

and $B = \Phi(v) = a(v) + a^\dagger(v)$. As already mentioned in the introduction, the commutator method of Lieb–Yamazaki (recalled in Appendix A) shows that under Assumption 1, B is infinitesimally form-bounded with respect to $|P - \mathbb{P}_f|^2 + d\Gamma(\omega)$, and in particular $\|C\| < 1$ for a large enough, where $C = A^{-1/2}(A + B)A^{-1/2} - 1$.

With Ω the vacuum state, we have $A\Omega = (|P|^2 + a)\Omega$. From (2.5), we thus obtain the convergent expansion

$$\begin{aligned} \langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle &= e^{ta} \langle \Omega | e^{-t(A+B)} \Omega \rangle \\ &= e^{-t|P|^2} + \sum_{n \geq 1} \frac{e^{ta}}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} \frac{e^{-tz}}{z - |P|^2 - a} \langle \Omega | \left(C \frac{A}{z - A} \right)^{2n} \Omega \rangle dz. \end{aligned} \quad (3.2)$$

Here, we used that only even n in (2.5) contribute, the odd terms have zero vacuum expectation value (since they necessarily involve an unequal number of creation and annihilation operators).

Let $C^+ = A^{-1/2}a^\dagger(v)A^{-1/2}$ and $C^- = A^{-1/2}a(v)A^{-1/2}$, so that $C = C^+ + C^-$. We have

$$\langle \Omega | \left(C \frac{A}{z - A} \right)^{2n} \Omega \rangle = \sum_{v \in \mathcal{D}_n} \langle \Omega | \prod_{j=1}^{2n} \left(C^{v_j} \frac{A}{z - A} \right) \Omega \rangle \quad (3.3)$$

where we identify $C^{+1} \equiv C^+$ and $C^{-1} \equiv C^-$, and $\mathcal{D}_n$ denotes the set of Dyck paths of length $2n$, i.e.,

$$\mathcal{D}_n = \left\{ v \in \{-1, +1\}^{2n} : \sum_{j=1}^k v_j \leq 0 \text{ for } 1 \leq k \leq 2n-1, \sum_{j=1}^{2n} v_j = 0 \right\}. \quad (3.4)$$

Only these terms contribute to the sum in (3.3), since particles can be annihilated only after they have been created, i.e., for a particle annihilated at step j , there had to be one created at some step $j' < j$. See Figure 2 for an illustration of a Dyck pack.

For $v \in \mathcal{D}_n$ for some $n \geq 1$, let

$$\Lambda_z(v) = \langle \Omega | \prod_{j=1}^{2n} \left(C^{v_j} \frac{A}{z - A} \right) \Omega \rangle. \quad (3.5)$$

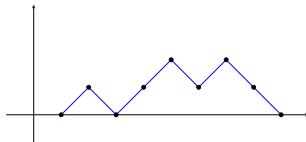


Fig. 2 Example of a Dyck path of length $2n = 8$, corresponding to $\nu = \{-1, +1, -1, -1, +1, -1, +1, +1\}$. Read from the right, we represent a creation (+1) with a line going up in the Dyck path, and an annihilation (-1) with a line going down

From (3.2)–(3.3), we thus have

$$\langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle = e^{-t|P|^2} + \sum_{v \in \mathcal{D}} \frac{e^{ta}}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} \frac{e^{-tz}}{z - |P|^2 - a} \Lambda_z(v) dz. \quad (3.6)$$

To compute the terms on the right-hand side, we need some further notation. Recall that $\mathcal{W}_{2n} \subset S_{2n}$ denotes the set of those permutations satisfying the Wick rule, i.e., $\pi(2j-1) < \pi(2j+1)$ for $j \in \{1, \dots, n-1\}$ and $\pi(2j-1) < \pi(2j)$ for $j \in \{1, \dots, n\}$. Recall also the definition of $\mathcal{E}_P^{(\pi, j)}$ in (1.4), and let

$$\mathcal{S}_P^\pi(z, \underline{k}) = \prod_{j=1}^{2n} \left(z - a - \mathcal{E}_P^{(\pi, j)}(\underline{k}) \right)^{-1} \quad (3.7)$$

for $\pi \in \mathcal{W}_{2n}$ and $\underline{k} = (k_1, \dots, k_n)$.

Lemma 1 Under Assumption 1,

$$\sup_{z \in \Gamma_{\gamma, \kappa}} \int_{\mathbb{R}^{dn}} |\mathcal{S}_P^\pi(z, \underline{k})| \prod_{j=1}^n |v(k_j)|^2 dk_j < \infty \quad (3.8)$$

for any $\pi \in \mathcal{W}_{2n}$ and $\gamma, \kappa > 0$.

Proof Recall the definition of $\mathcal{M}_j^\pi$ in (1.3). A little thought reveals that, for any $1 \leq j \leq 2n$, $\mathcal{M}_{j-1}^\pi$ and $\mathcal{M}_j^\pi$ differ by exactly one element, namely, the $i \in \{1, \dots, n\}$ such that $j \in \{\pi(2i-1), \pi(2i)\}$. We shall denote it by i_j . With the aid of (2.8), one readily finds that

$$\left| \left(z - a - \mathcal{E}_P^{(\pi, j-1)}(\underline{k}) \right) \left(z - a - \mathcal{E}_P^{(\pi, j)}(\underline{k}) \right) \right| \geq \frac{(\kappa + a)(\kappa + a + \omega(k_{i_j}) + \frac{1}{2}|k_{i_j}|^2)}{1 + \gamma^2} \quad (3.9)$$

for $z \in \Gamma_{\gamma, \kappa}$ and $1 \leq j \leq 2n$. Since $\mathcal{M}_0^\pi = \mathcal{M}_{2n}^\pi = \emptyset$ and thus $\mathcal{E}_P^{\pi, 0} = \mathcal{E}_P^{\pi, 2n} = |P|^2$, we can write

$$|\mathcal{S}_P^\pi(z, \underline{k})| = \prod_{j=1}^{2n} \left| z - a - \mathcal{E}_P^{(\pi, j-1)}(\underline{k}) \right|^{-1/2} \left| z - a - \mathcal{E}_P^{(\pi, j)}(\underline{k}) \right|^{-1/2} \quad (3.10)$$

and hence, (3.9) yields the bound

$$|\mathcal{S}_P^\pi(z, \underline{k})| \leq \left(\frac{1 + \gamma^2}{\kappa + a} \right)^n \prod_{j=1}^{2n} \left(\kappa + a + \omega(k_{i_j}) + \frac{1}{2}|k_{i_j}|^2 \right)^{-1/2}. \quad (3.11)$$

By construction, each k_i appears exactly twice in the list $\{k_{i_1}, \dots, k_{i_{2n}}\}$, hence (3.11) reads

$$|\mathcal{S}_P^\pi(z, \underline{k})| \leq \left(\frac{1 + \gamma^2}{\kappa + a} \right)^n \prod_{i=1}^n \frac{1}{\kappa + a + \omega(k_i) + \frac{1}{2}|k_i|^2}. \quad (3.12)$$

The claim (3.8) then follows from our assumptions on v and ω in Assumption 1. $\square$

Each Wick pairing $\pi \in \mathcal{W}_{2n}$ corresponds to a Dyck path defined by $v_{\pi(j)} = (-1)^j$. We can thus decompose $\mathcal{W}_{2n} = \bigcup_{v \in \mathcal{D}_n} \mathcal{W}_{2n}^v$, where $\mathcal{W}_{2n}^v \subset \mathcal{W}_{2n}$ denotes the set of those Wick pairings giving rise to the same Dyck path v . With this notation, we have the following identity for $\Lambda_z(v)$ defined in (3.5).

Lemma 2 *Under Assumption 1, we have*

$$\Lambda_z(v) = \sum_{\pi \in \mathcal{W}_{2n}^v} \int_{\mathbb{R}^{dn}} \mathcal{S}_P^\pi(z, \underline{k}) \prod_{j=1}^n |v(k_j)|^2 dk_j \quad (3.13)$$

for any $v \in \mathcal{D}_n$ and $z \in \Gamma_{\gamma, \kappa}$.

Formally, the identity (3.13) follows from an application of the Wick rule and the pull-through formula $a_k \mathcal{R}(\mathrm{d}\Gamma(\omega), \mathbb{P}_f) = \mathcal{R}(\mathrm{d}\Gamma(\omega) + \omega(k), \mathbb{P}_f + k) a_k$ for functions $\mathcal{R}$ and the operator-valued distribution a_k used to define $a(v)$ by $a(v) = \int a_k \overline{v(k)} dk$. The proof below can be viewed as a rigorous justification of this procedure.

Proof By analyticity and the uniform integrability established in Lemma 1, it suffices to consider the case $\Re z < 0$. Moreover, since both sides of (3.13) are continuous in v (with respect to the norm defined in Assumption 1), it suffices to consider the case of suitably nice v . We shall in fact first assume that $k \mapsto v(k)e^{s\omega(k)}$ is in $L^2(\mathbb{R}^d)$ for any $s > 0$. In particular, we work under the assumption $v \in L^2(\mathbb{R}^d)$, in which case $a(v)$ is effectively a bounded operator in our computations (where the number of particles is bounded by n). Moreover, if ω is unbounded, this assumption additionally requires v to suitably decay. (We could choose it to have compact support, for instance.) For $\Re z < 0$ we can write

$$\frac{1}{z - A} = - \int_0^\infty \frac{e^{s(z-A)}}{(4\pi s)^{d/2}} e^{-s\mathrm{d}\Gamma(\omega)} \int_{\mathbb{R}^d} e^{ip \cdot (P - \mathbb{P}_f)} e^{-|p|^2/(4s)} dp ds \quad (3.14)$$

and hence

$$\Lambda_z(v) = \left\langle \Omega \left| \prod_{j=1}^{2n} \left(a^{v_j}(v) \frac{1}{z - A} \right) \Omega \right. \right\rangle$$

$$\begin{aligned}
&= \int_{\mathbb{R}_+^{2n} \times \mathbb{R}^{2nd}} \prod_{j=1}^{2n} \frac{e^{s_j(z-a)}}{(4\pi s_j)^{d/2}} e^{ip_j \cdot P} e^{-|p_j|^2/(4s_j)} \\
&\quad \times \langle \Omega | \prod_{j=1}^{2n} \left(a^{v_j}(v) e^{-s_j d\Gamma(\omega)} e^{-ip_j \cdot \mathbb{P}_f} \right) \Omega \rangle \prod_{j=1}^{2n} ds_j dp_j \quad (3.15)
\end{aligned}$$

where we identify $a^-(v) = a(v)$ and $a^+(v) = a^\dagger(v)$. Moreover, since

$$e^{-sd\Gamma(\omega)} e^{-ip \cdot \mathbb{P}_f} a^v(v) = a^v(e^{-sv\omega} e^{-ip \cdot v}) e^{-sd\Gamma(\omega)} e^{-ip \cdot \mathbb{P}_f} \quad (3.16)$$

for $v \in \{+, -\}$, we have

$$\left\langle \Omega \left| \prod_{j=1}^{2n} \left(a^{v_j}(v) e^{-s_j d\Gamma(\omega)} e^{-ip_j \cdot \mathbb{P}_f} \right) \Omega \right. \right\rangle = \left\langle \Omega \left| \prod_{j=1}^{2n} a^{v_j}(v_j) \Omega \right. \right\rangle \quad (3.17)$$

with $v_1 = v$ and

$$v_j(k) = v(k) e^{-\omega(k)v_j \sum_{\ell=1}^{j-1} s_\ell} e^{-ik \cdot \sum_{\ell=1}^{j-1} p_\ell} \quad (3.18)$$

for $j \geq 2$. An application of Wick's rule further yields

$$\begin{aligned}
\left\langle \Omega \left| \prod_{j=1}^{2n} a^{v_j}(v_j) \Omega \right. \right\rangle &= \sum_{\pi \in \mathcal{W}_{2n}} \prod_{i=1}^n \left\langle \Omega \left| a^{v_{\pi(2i-1)}}(v_{\pi(2i-1)}) a^{v_{\pi(2i)}}(v_{\pi(2i)}) \Omega \right. \right\rangle \\
&= \sum_{\pi \in \mathcal{W}_{2n}} \prod_{i=1}^n \left\langle v_{\pi(2i-1)} \left| v_{\pi(2i)} \right. \right\rangle \delta_{v_{\pi(2i-1)}, -1} \delta_{v_{\pi(2i)}, +1} \\
&= \sum_{\pi \in \mathcal{W}_{2n}^v} \prod_{i=1}^n \left\langle v_{\pi(2i-1)} \left| v_{\pi(2i)} \right. \right\rangle \\
&= \sum_{\pi \in \mathcal{W}_{2n}^v} \prod_{i=1}^n \int_{\mathbb{R}^d} |v(k)|^2 e^{-\omega(k) \sum_{\ell=\pi(2i-1)}^{\pi(2i)-1} s_\ell} e^{-ik \cdot \sum_{\ell=\pi(2i-1)}^{\pi(2i)-1} p_\ell} dk. \quad (3.19)
\end{aligned}$$

Inserting this in (3.15) above and interchanging the order of integrations then gives the desired formula (3.13) under the stated assumptions on v , i.e., under the assumption that $k \mapsto v(k) e^{s\omega(k)}$ is in $L^2(\mathbb{R}^d)$ for any $s > 0$. The set of such v 's can easily be seen to be dense in the set defined by Assumption 1 for the appropriate norm; hence, the general case follows by continuity of both sides of (3.13), as already mentioned in the beginning of the proof. $\square$

We now have all the prerequisites to give the proof of our main results.

4 Proof of the main results

4.1 Proof of Theorem 1(a)

The starting point is (3.6), where we insert the identity (3.13) from Lemma 2. Because of the uniform integrability established in Lemma 1, we can interchange the integration over $k_1, \dots, k_n$ with the one over z and do the latter first. One easily checks that for positive numbers b_j , one has

$$\frac{1}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} e^{-tz} \prod_{j=0}^{2n} \frac{1}{z - b_j} dz = \int_{\Delta_{2n}^t} e^{-\sum_{j=0}^{2n} t_j b_j} d\mathbf{t}_- \quad (4.1)$$

(To see this, send $\gamma \rightarrow 0$, and write $(z - b_j)^{-1} = -\int_0^\infty e^{s(z-b_j)} ds$ for $z \in \Gamma_{0, \kappa} = \{-\kappa + it : t \in \mathbb{R}\}$, as sketched by the red contour in Figure 1.) In particular, for $\mathcal{S}_P^\pi$ in (3.7)

$$\frac{e^{ta}}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} \frac{e^{-tz}}{z - |P|^2 - a} \mathcal{S}_P^\pi(z, \underline{k}) dz = \int_{\Delta_{2n}^t} e^{-\sum_{j=0}^{2n} t_j \mathcal{E}_P^{(\pi, j)}(\underline{k})} d\mathbf{t}_- \quad (4.2)$$

using again that $\mathcal{E}_P^{(\pi, 0)} = |P|^2$. By positivity of the integrand, we can exchange the integration over $\mathbf{t}_-$ with the one over $\underline{k}$, thus arriving at the desired expansion (1.6). $\square$

4.2 Proof of Corollary 1(a)

By Bernstein's Theorem, Assumption 2 implies that for any $r, s > 0$ there exists a measure on $d\mu_{r,s}$ on $\mathbb{R}_+$ such that

$$\int_{\mathbb{R}^d} e^{-r|P-k|^2 - s\omega(k)} |v(k)|^2 dk = \int_0^\infty e^{-\lambda|P|^2} d\mu_{r,s}(\lambda). \quad (4.3)$$

We claim that this implies, for any $n \geq 1$,

$$\int_{\mathbb{R}^{dn}} e^{-Q(P, \underline{k})} \prod_{j=1}^n e^{-s_j \omega(k_j)} |v(k_j)|^2 dk_j = \int_0^\infty e^{-\lambda|P|^2} d\mu_{Q, \underline{s}}(\lambda) \quad (4.4)$$

for a suitable measure $d\mu_{Q, \underline{s}}$, for any set of positive parameters $\underline{s} = (s_1, \dots, s_n) \in \mathbb{R}_+^n$ and any positive quadratic form Q on $\mathbb{R}^{d(n+1)}$ that is invariant under simultaneous rotations of the $n+1$ variables, i.e., is of the form $Q(k_0, \underline{k}) = \sum_{i,j=0}^n Q_{ij} k_i \cdot k_j$ for a positive symmetric matrix with coefficients Q_{ij} .

In the case $n=1$, this follows readily from (4.3), since $Q(P, k_1)$ can be written as $Q_{11}|k_1| + Q_{01}Q_{11}^{-1}|P|^2 + (Q_{00} - Q_{01}^2 Q_{11}^{-1})|P|^2$.

For general n , we can proceed by induction. Singling out the last integration variable k_n , we can write

$$\mathcal{Q}(k_0, \underline{k}) = \mathcal{Q}_{nn} \left| k_n + \mathcal{Q}_{nn}^{-1} \sum_{j=0}^{n-1} \mathcal{Q}_{jn} k_j \right|^2 + \mathcal{Q}'(k_0, k_1, \dots, k_{n-1}) \quad (4.5)$$

with $\mathcal{Q}'$ a rotation-invariant non-negative quadratic form on $\mathbb{R}^{dn}$, given by

$$\mathcal{Q}'_{ij} = \mathcal{Q}_{ij} - \frac{1}{\mathcal{Q}_{nn}} \mathcal{Q}_{in} \mathcal{Q}_{nj} \quad \text{for } 0 \leq i, j \leq n-1. \quad (4.6)$$

Applying (4.3) to the integration over k_n , we are left with an integral over similar problems for $n-1$ variables, with quadratic expressions $\lambda |\mathcal{Q}_{0n} P + \sum_{j=1}^{n-1} \mathcal{Q}_{jn} k_j|^2 + \mathcal{Q}'(P, k_1, \dots, k_{n-1})$ for $\lambda \geq 0$. The claim (4.4) thus follows by induction.

By positivity of the integrand, we can first carry out the integration over $\underline{k}$ for fixed $\underline{t}$ in the various terms in (1.6). For given $\underline{t} = (t_0, \dots, t_{2n}) \in \mathbb{R}_+^{2n+1}$ and $\pi \in \mathcal{W}_{2n}$, the function $\sum_{j=0}^{2n} t_j \mathcal{E}_P^{(\pi, j)}(\underline{k})$ is of the form

$$\sum_{j=0}^{2n} t_j \mathcal{E}_P^{(\pi, j)}(\underline{k}) = \mathcal{Q}(P, \underline{k}) + \sum_{j=1}^n s_j \omega(k_j) \quad (4.7)$$

for a rotation-invariant positive quadratic form $\mathcal{Q}$ and positive parameters s_j . The claimed complete monotonicity is thus an immediate consequence of (4.4). $\square$

4.3 Proof of Theorem 1(b)

The starting point is again (3.6), but we shall change back the order of integration and summation (which is allowed for small enough γ , as shown in the proof of Theorem 2 in Sect. 2). That is, we have

$$\left\langle \Omega \left| e^{-t\mathbb{H}(P)} \Omega \right. \right\rangle = e^{-t|P|^2} + \frac{e^{t\alpha}}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} \frac{e^{-tz}}{z - |P|^2 - \alpha} \sum_{v \in \mathcal{D}} \Lambda_z(v) dz. \quad (4.8)$$

Recall the definition of the Dyck paths $\mathcal{D}_n$ in (3.4), and the one of Λ_z in (3.5). Given $v \in \mathcal{D}_n$ and $v' \in \mathcal{D}_{n'}$, we can concatenate them to $\{v, v'\} \in \mathcal{D}_{n+n'}$. We have

$$\Lambda_z(\{v, v'\}) = \Lambda_z(v) \Lambda_z(v') \quad (4.9)$$

and, if we set $\Lambda_z(\emptyset) = 1$, this continues to hold for $v = \emptyset$. Every $v \in \mathcal{D}_n$ can be uniquely written as $v = \{\tilde{v}, v_0\}$ where $v_0 \in \mathcal{D}_m^0$ for some $1 \leq m \leq n$ and $\tilde{v} \in \mathcal{D}_{n-m}$ (being possibly empty), where $\mathcal{D}_n^0 \subset \mathcal{D}_n$ denotes those Dyck paths that return to the origin only at the end, i.e., satisfy $\sum_{j=1}^k v_j < 0$ for all $1 \leq k \leq 2n-1$. Hence, with

$\mathcal{D} = \bigcup_{n \geq 1} \mathcal{D}_n$ (and similarly for $\mathcal{D}^0$)

$$\sum_{v \in \mathcal{D}} \Lambda_z(v) = \left(1 + \sum_{\tilde{v} \in \mathcal{D}} \Lambda_z(\tilde{v})\right) \sum_{v_0 \in \mathcal{D}^0} \Lambda_z(v_0). \quad (4.10)$$

For two functions f_1 and f_2 analytic away from the positive half-line (and satisfying suitable growth bounds), we have

$$\begin{aligned} & \frac{1}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} e^{-tz} f_1(z) f_2(z) dz \\ &= \int_0^t \left(\frac{1}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} e^{-(t-s)z} f_1(z) dz \right) \left(\frac{1}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} e^{-sz'} f_2(z') dz' \right) ds. \end{aligned} \quad (4.11)$$

We shall apply this with $f_1(z) = (z - |P|^2 - a)^{-1} (1 + \sum_{v \in \mathcal{D}} \Lambda_z(v))$ and $f_2(z) = \sum_{v \in \mathcal{D}^0} \Lambda_z(v)$. Using also (4.8) with t replaced by s , we find

$$\left\langle \Omega \left| e^{-t\mathbb{H}(P)} \Omega \right. \right\rangle = e^{-t|P|^2} + \int_0^t \left\langle \Omega \left| e^{-(t-s)\mathbb{H}(P)} \Omega \right. \right\rangle \frac{e^{sa}}{2\pi i} \int_{\Gamma_{\gamma, \kappa}} e^{-sz} \sum_{v \in \mathcal{D}^0} \Lambda_z(v) dz ds. \quad (4.12)$$

Lemma 2 implies that

$$\sum_{v \in \mathcal{D}_n^0} \Lambda_z(v) = \sum_{\pi \in \mathcal{W}_{2n}^0} \int_{\mathbb{R}^{dn}} \mathcal{S}_P^\pi(z, \underline{k}) \prod_{j=1}^n |v(k_j)|^2 dk_j \quad (4.13)$$

where $\mathcal{W}_{2n}^0 \subset \mathcal{W}_{2n}$ are those Wick pairings such that $j \mapsto (-1)^{\pi^{-1}(j)}$ is in $\mathcal{D}_n^0$, which are precisely the interlacing Wick pairings defined in the introduction. The desired identity (1.7) then follows by proceeding as in Sect. 4.1 (compare with (4.2)). $\square$

4.4 Proof of Corollary 1(b)

As already mentioned in the introduction, concavity of $|P|^2 \mapsto E_0(P)$ is an immediate consequence of part (a) in combination with (1.12).

For $v \neq 0$, a simple variational argument shows that $E_0(P) < |P|^2$ for all $P \in \mathbb{R}^d$. If we assume that $\mathbb{H}(P)$ has a ground state Φ_P , then

$$\lim_{t \rightarrow \infty} e^{tE_0(P)} \langle \Omega | e^{-t\mathbb{H}(P)} \Omega \rangle = |\langle \Omega | \Phi_P \rangle|^2 > 0 \quad (4.14)$$

where the strict positivity follows from the fact that $e^{-t\mathbb{H}(P)}$ is positivity improving on a suitable cone containing the vacuum [11]. (The statement is proved in [11] for the Fröhlich model, but the method of proof applies to the general case considered here.)

We can thus take $t \rightarrow \infty$ in (1.7) and obtain, using dominated convergence,

$$1 = \int_0^\infty e^{sE_0(P)} \sum_{n \geq 1} \sum_{\pi \in \mathcal{W}_{2n}^0} \int_{\Delta_{2n-1}^s} \int_{\mathbb{R}^{dn}} e^{-\sum_{j=0}^{2n-1} t_j \mathcal{E}_P^{(\pi,j)}(k)} \prod_{j=1}^n |v(k_j)|^2 dk_j d\underline{t} ds. \quad (4.15)$$

From the complete monotonicity of the terms multiplying $e^{sE_0(P)}$ in the integrand, it is then easy to see that Hölder's inequality implies that $|P|^2 \mapsto E_0(P)$ is strictly concave (as argued in [14, Cor. 8]), using again Bernstein's theorem. $\square$

Appendix A: the Lieb–Yamazaki argument

In this section, we shall recall the Lieb–Yamazaki commutator method introduced in [10, Sect. 2] to prove that if v and ω satisfy Assumption 1, $\Phi(v)$ is infinitesimally form-bounded with respect to the non-interacting Hamiltonian $|P - \mathbb{P}_f|^2 + d\Gamma(\omega)$. On the one hand, a simple Cauchy–Schwarz inequality shows that

$$\pm \Phi(v) \leq \varepsilon d\Gamma(\omega) + \varepsilon^{-1} \int_{\mathbb{R}^d} \frac{|v(k)|^2}{\omega(k)} dk \quad (A.1)$$

for any $\varepsilon > 0$, which we can apply to $v = v_1$. On the other hand, using that

$$\Phi(v) = i[P - \mathbb{P}_f, \Phi(w)] \quad (A.2)$$

for $w(k) = ikv(k)/|k|^2$ (where an inner product between the vectors $P - \mathbb{P}_f$ and w is understood on the right-hand side), a Cauchy–Schwarz inequality implies that

$$\pm \Phi(v) \leq \varepsilon |P - \mathbb{P}_f|^2 + \varepsilon^{-1} |\Phi(w)|^2. \quad (A.3)$$

We can further bound

$$\Phi(w)^2 \leq 4a^\dagger(w)a(w) + 2\|w\|^2 \leq \lambda d\Gamma(\omega) + 2 \int_{\mathbb{R}^d} \frac{|v(k)|^2}{|k|^2} dk \quad (A.4)$$

for $\lambda = 4 \int |w(k)|^2/\omega(k) dk = 4 \int |v(k)|^2/(|k|^2 \omega(k)) dk$. We shall apply this bound to v_2 . By suitably adjusting how to split v into the two components $v = v_1 + v_2$, we can assume that λ is as small as desired, which implies the claimed infinitesimal bound relative to $|P - \mathbb{P}_f|^2 + d\Gamma(\omega)$.

Funding Open access funding provided by Institute of Science and Technology (IST Austria).

Declarations

Conflict of interest The authors have no relevant financial or non-financial interests to disclose. No datasets were generated or analyzed during the current study.

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