Occupation Density

Abstract

The

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1 Introduction

We consider a quantum system of N spinless fermionic particles on $\mathbb{T} := [0, 2\pi]^3$. The system is described by the Hamiltonian

$$H = -\hbar^2 \sum_{j=1}^{N} \Delta_{x_j} + \lambda \sum_{1 \leq i < j \leq N} V(x_i - x_j) \tag{1}$$

acting on the wave functions in the anti-symmetric tensor product $L^2_a(\mathbb{T}^{3N}) = \bigwedge_{i=1}^{N} L^2_a(\mathbb{T}^3)$. We want to find the occupation density in the asymptotic limit when $N \to \infty$ in the *mean-field scaling regime* i.e. we set

$$\hbar := N^{-\frac{1}{3}}, \quad \text{and} \quad \lambda := N^{-1} \tag{2}$$

Then we have

$$\langle \Psi_{trial}, n_q \Psi_{trial} \rangle = \left\langle \Psi_{trial}, a_q^* a_q \Psi_{trial} \right\rangle \tag{3}$$

2 Computations

Consider a trial state Ψ_{trial} such that $\langle \Psi_{trial}, H\Psi_{trial} \rangle = E_{HF} + E_{RPA} + o(\hbar)$, where E_{HF} is the Hartree-Fock energy and E_{RPA} is the correlation energy from RPA.

We need to calculate $\langle \Psi_{trial}, a_l^* a_l \Psi_{trial} \rangle$, $l \in \mathbb{Z}^3$. (Correct all ls to ℓ) Here the trial state $\Psi_{trial} = Re^k\Omega$, where

$$R\Omega = \frac{1}{\sqrt{N!}} \det \left(\frac{1}{(2\pi)^{3/2}} e^{ik_j \cdot x_i} \right)_{j,i=1}^{N}. \tag{4}$$

is the Slater determinant of all plane waves with N different momenta $k_j \in \mathbb{Z}^3$. We have the Fermi ball i.e. states filling up all the momenta up to Fermi momentum as

$$B_F := \left\{ k \in \mathbb{Z}^3 : |k| \leq k_F \right\} \tag{5}$$

for some $k_F > 0$ and we define its complement as

$$B_F^c = \mathbb{Z}^3 \setminus B_F \tag{6}$$

Similarly we define a set of momenta which are outside the Fermi ball but are constrained to be a certain distance away from the Fermi ball as

$$L_q \coloneqq \{p : p \in B_F^c \cap (B_F + k)\} \tag{7}$$

with the following symmetry $L_{-k} = -L_k \quad \forall k \in \mathbb{Z}^3$.

We define the pair operators as

$$b_p(k) = a_{p-k} a_p \tag{8}$$
$$b_p^*(k) = a_p^* a_{p-k}^* \tag{9}$$

for $p \in L_k$

Lemma 2.1 (Quasi-Bosonic commutation relation)**.**

$$[b_p(k), b_q(\ell)] = [b_p^*(k), b_q^*(\ell)] = 0 \tag{10}$$
$$[b_p(k), b_q^*(\ell)] = \delta_{p,q}\delta_{k,l} + \epsilon_{p,q}(k,l), \tag{11}$$

where $\epsilon_{p,q}(k,l) = -\left(\delta_{p,q} a_{q-l}^* a_{p-k} + \delta_{p-k,q-l} a_q^* a_p\right)$

Proof.

$$\begin{aligned} [b_p(k), b_q^*(\ell)] &= [a_{p-k} a_p, a_q^* a_{q-l}^*] && (12)\\ &= a_{p-k}[a_p, a_q^* a_{q-l}^*] + [a_{p-k}, a_q^* a_{q-l}^*] a_p && (13)\\ &= a_{p-k}\left\{a_p, a_q^*\right\} a_{q-l}^* - a_{p-k} a_q^* \{a_p, a_{q-l}^*\} \\ &+ \{a_{p-k}, a_q^*\} a_{q-l}^* a_p - a_q^* \{a_{p-k}, a_{q-l}^*\} a_p && (14)\\ &= \delta_{p,q} a_{p-k} a_{q-l}^* + \delta_{p-k,q-l} a_q^* a_p && (15)\\ &= \delta_{p,q}\delta_{k,l} - \left(\delta_{p,q} a_{q-l}^* a_{p-k} + \delta_{p-k,q-l} a_q^* a_p\right) && (16) \end{aligned}$$

Here, we denote the error term as $\epsilon_{p,q}(k,l) = -\left(\delta_{p,q} a_{q-l}^* a_{p-k} + \delta_{p-k,q-l} a_q^* a_p\right)$ with $\epsilon_{p,p}(k,k) \geq 0$ □

Before we more on we write some more commutation relation in order to facilitate further computations.

Lemma 2.2 (Commutation relation between $a_p^\sharp$,[1] and n_q)**.**

$$\left[n_q, a_p^*\right] = \delta_{q.p} a_p^* \tag{17}$$
$$[n_q, a_p] = -\delta_{q.p} a_p \tag{18}$$

Proof.

$$\begin{aligned} \left[n_q, a_p^*\right] &= \left[a_q^* a_q, a_p^*\right] && (19)\\ &= a_q^* a_q a_p^* - a_p^* a_q^* a_q && (20)\\ &= a_q^* \delta_{qp} - a_q^* a_p^* a_q - a_p^* a_q^* a_q && (21)\\ &= \delta_{q,p} a_p^* && (22) \end{aligned}$$

Here the second step follows from CAR for the fermionic creation and annihilation operators.

[1] Here $\sharp = \{\ , *\}$

For the second commutation relation, we observe that

$$[n_q, a_p] = - \left[n_q, a_p^*\right]^* \tag{23}$$

Hence the commutation relation holds □

Lemma 2.3 (Commutation relation between $b_p^\sharp$ and n_q)**.**

$$\left[n_q, b_p^*(k)\right] = \left(\delta_{q.p} + \delta_{q.p-k}\right) b_p^*(k) \tag{24}$$
$$[n_q, b_p(k)] = - \left(\delta_{q.p} + \delta_{q.p-k}\right) b_p(k) \tag{25}$$

Proof. To be filled in □

Consider a set of symmetric operator $K(\ell) : \ell^2(L_l) \to \ell^2(L_l), l \in \mathbb{Z}_*^3$. Then we define the associated Bogoliubov kernel $\mathcal{K} : \mathcal{H}_N \to \mathcal{H}_N$ by

$$\mathcal{K} = \frac{1}{2} \sum_{l \in \mathbb{Z}_*^3} \sum_{r,s \in L_l} K(\ell)_{r,s} \left(b_r(\ell) b_{-s}(-\ell) - b_{-s}^*(-\ell) b_r^*(\ell)\right) \tag{26}$$

Next we define the transformation $T = e^{\mathcal{K}}$ which is a unitary due the fact that $\mathcal{K}$ is anti-unitary i.e. $\mathcal{K} = -\mathcal{K}^*$.

For further convenience, we write the following commutation relation.

Lemma 2.4 (Commutator between $\mathcal{K}$ and pair operators)**.**

$$[\mathcal{K}, b_p^*(k)] = \sum_{s \in L_k} K(k)_{p,s} b_{-s}(-k) + \mathcal{E}_p(k) \tag{27}$$
$$[\mathcal{K}, b_p(k)] = \sum_{s \in L_k} K(k)_{p,s} b_{-s}^*(-k) + \left(\mathcal{E}_p(k)\right)^*, \tag{28}$$

where,

$$\mathcal{E}_p(k) = \frac{1}{2} \sum_{l \in \mathbb{Z}_*^3} \sum_{r,s \in L_l} K(\ell)_{r,s} \left\{b_r(\ell), \epsilon_{-s,p}(k, -l)\right\} \tag{29}$$

Proof. to be filled in □

Before we begin the evaluation, we define .

Symmetry transformation Symmetry transformation is a unitary transformation $\mathfrak{R} : \mathcal{F} \to \mathcal{F}$ defined by its action as

$$\mathfrak{R} : a_{k_1}^* \dots a_{k_n}^* \Omega \mapsto a_{-k_1}^* \dots a_{-k_n}^* \Omega \tag{30}$$

while leaving the vacuum state invariant.

Lemma 2.5. *For the symmetry transformation $\mathfrak{R}$ and the almost bosonic Bogoliubov transformation T, we have*

$$\mathfrak{R} T \Omega = T \Omega \tag{31}$$

Proof. to be filled in □

Next we define the quadratic operator as

Definition 2.6. For $l \in \mathbb{Z}_*^3$

$$Q_1(A(\ell)) \coloneqq \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_l} A(\ell)_{r,s} \left(b_r^*(\ell) b_s(\ell) + b_s^*(\ell) b_r(\ell)\right) \tag{32}$$
$$Q_2(A(\ell)) \coloneqq \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_l} A(\ell)_{r,s} \left(b_r(\ell) b_{-s}(-\ell) + b_{-s}^*(-\ell) b_r^*(\ell)\right) \tag{33}$$

Then motivated by Lemma 2.5, we evaluate $\left\langle \Omega, T_1^* \frac{1}{2}\left(n_q + n_{-q}\right) T_1 \Omega \right\rangle$.

Evaluation of the expectation value

Lemma 2.7. *For $q \in B_F^c$, we define the projection operator, projecting to momentum q and $-q$, $(\Delta^q)_{m,s} := -\frac{1}{2}(\delta_{m,q}\delta_{m,s} + \delta_{m,-q}\delta_{m.s})$ and we get*

$$\left\langle \Omega, T_1^* \frac{1}{2}\left(n_q + n_{-q}\right) T_1 \Omega \right\rangle = \tag{34}$$

Proof. We start by applying Duhamel's formula to RHS of (34) and we have

$$\frac{1}{2}\left(\left\langle \Omega, \left(n_q + n_{-q}\right) \Omega \right\rangle + \int_0^1 d\lambda \left(\frac{d}{d\lambda} \left\langle \Omega, T_\lambda^* \left(n_q + n_{-q}\right) T_\lambda \Omega \right\rangle \right) \right) \tag{35}$$

$$= \frac{1}{2} \int_0^1 d\lambda \left(\left\langle \Omega, T_\lambda^* (-\mathcal{K}) \left(n_q + n_{-q}\right) T_\lambda + T_\lambda^* \left(n_q + n_{-q}\right) (\mathcal{K}) T_\lambda \Omega \right\rangle \right) \tag{36}$$

$$= \frac{1}{2} \int_0^1 d\lambda \left\langle \Omega, T_\lambda^* [\left(n_q + n_{-q}\right), \mathcal{K}] T_\lambda \Omega \right\rangle . \tag{37}$$

Next using the definition of $\mathcal{K}$, we write the expression for the commutator.

$$[n_q, \mathcal{K}] = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \left[a_q^* a_q, \left(b_r(\ell) b_{-s}(-\ell) - b_{-s}^*(-\ell) b_r^*(\ell) \right) \right] \tag{38}$$

$$\begin{aligned} = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big(& \left[a_q^* a_q, b_r(\ell) \right] b_{-s}(-\ell) + b_r(\ell) \left[a_q^* a_q, b_{-s}(-\ell) \right] \\ & - \left[a_q^* a_q, b_{-s}^*(-\ell) \right] b_r^*(\ell) + b_{-s}^*(-\ell) \left[a_q^* a_q, b_r^*(\ell) \right] \Big) \end{aligned} \tag{39}$$

$$\begin{aligned} = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big(& (-1) \left(\delta_{q.r} + \delta_{q.r-\ell} + \delta_{q,-s} + \delta_{q,-s+\ell} \right) \\ & \times \left(b_r(\ell) b_{-s}(-\ell) + b_{-s}^*(-\ell) b_r^*(\ell) \right) \Big) \end{aligned} \tag{40}$$

Now, since $q \in B_F^c$, $\delta_{q.r-\ell} = \delta_{q,-s+\ell} = 0$, we have

$$[n_q, \mathcal{K}] = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big((-1)(\delta_{q.r} + \delta_{q,-s}) \left(b_r(\ell) b_{-s}(-\ell) + b_{-s}^*(-\ell) b_r^*(\ell) \right) \Big) \tag{41}$$

Similarly for $[n_q, \mathcal{K}]$, we get

$$[n_{-q}, \mathcal{K}] = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big((-1)(\delta_{-q.r} + \delta_{-q,-s}) \left(b_r(\ell) b_{-s}(-\ell) + b_{-s}^*(-\ell) b_r^*(\ell) \right) \Big) \tag{42}$$

Next we substitute commutators (41) and (42) in (37),

$$
\begin{aligned}
(37) = \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* \Big(\frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big((-1)(\delta_{q.r} + \delta_{q,-s} + \delta_{-q.r} + \delta_{-q,-s}) \\
\times (b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)) \Big) \Big) T_\lambda \Omega \Big\rangle \\
= \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} (-\frac{1}{2}) \Big(\underbrace{K(\ell)_{r,s}(\delta_{q.r} + \delta_{q,-s} + \delta_{-q.r} + \delta_{-q,-s})}_{\text{interpret as matrix product}} \\
\times (b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)) \Big) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{43}
$$

$$
\begin{aligned}
= \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big(K(\ell)_{r,m} (-\frac{1}{2}) \underbrace{(\delta_{m,q}\delta_{m,s} + \delta_{m,-q}\delta_{m.s})}_{\text{(a)}} \\
+ (-\frac{1}{2}) \underbrace{(\delta_{r,q}\delta_{r,m} + \delta_{r,-q}\delta_{r.m})}_{\text{(b)}} K(\ell)_{m,s} \Big) (b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{44}
$$

Next, we observe that (a) and (b) are projection of a momentum (r or $s \in L_\ell$) to momentum q and $-q$. We then arrive at

$$
\begin{aligned}
(44) = \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big(K(\ell)_{r,m} \Delta^q_{m,s} + \Delta^q_{r,m} K(\ell)_{m,s} \Big) \qquad (45) \\
(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)) \Big) T_\lambda \Omega \Big\rangle \\
= \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big(K(\ell)_{r,m} \Delta^q_{m,s} + \Delta^q_{r,m} K(\ell)_{m,s} \Big) \qquad (46) \\
(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)) \Big) T_\lambda \Omega \Big\rangle \\
= \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big\{ K(\ell), \Delta^q \Big\}_{r,s} (b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{47}
$$

Using the definition of Q_2, (33), we arrive at

$$
(47) = \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* Q_2 \Big(\big\{ K(\ell), \Delta^q \big\} \Big) T_\lambda \Omega \Big\rangle \tag{48}
$$

□

Lemma 2.8 (Commutator between $\mathcal{K}$ and the quadratic operators)**.**

$$[Q_1(A(\ell)),\mathcal{K}] = Q_2(\{K(\ell),A(\ell)\}) + E_{Q_1}(A(\ell)) \tag{49}$$
$$[Q_2(B(\ell)),\mathcal{K}] = Q_1(\{K(\ell),B(\ell)\}) + E_{Q_2}(B(\ell)) \tag{50}$$

where,

$$E_{Q_1}(A(\ell)) = -\big(b_r(\ell)\mathcal{E}^*_{-s}(-\ell) + \mathcal{E}_r(\ell)b_{-s}(\ell) + \mathcal{E}_{-s}(-\ell)b^*_r(\ell) + b^*_{-s}(-\ell)\mathcal{E}^*_r(\ell)\big) \tag{51}$$
$$E_{Q_2}(B(\ell)) = -\big(b^*_r(\ell)\mathcal{E}^*_{-s}(-\ell) + \mathcal{E}_r(\ell)b_{-s}(\ell) + \mathcal{E}_{-s}(-\ell)b_r(\ell) + b^*_{-s}(-\ell)\mathcal{E}^*_r(\ell)\big) \tag{52}$$

Proof. We begin with $[Q_2(B_k),\mathcal{K}]$.
Some error in the indices

Similarly one can prove $[\mathcal{K},Q_1(A_k)]$. □

2.1 Transformation of quadratic operators

We begin with $T_1^*Q_!(A(\ell))T_1$ and apply Duhamel's formula,

$$T_1^*Q_1(A(\ell))T_1 = Q_1(A(\ell)) + \int_0^1 \frac{d}{d\lambda}\left(T_\lambda^*Q_1(A(\ell))T_\lambda\right)d\lambda \tag{53}$$
$$= Q_1(A_k) + \int_0^1 T_\lambda^*[\mathcal{K},Q_1(A_k)]T_\lambda d\lambda. \tag{54}$$

Then from the lemma above, we get

$$(54) = Q_1(A_k) + \int_0^1 T_\lambda^*(Q_2(\{K_k,A_k\}) + E_{Q_1}(K_k,A_k))T_\lambda d\lambda \tag{55}$$
$$= Q_1(A_k) + \int_0^1 T_\lambda^*(Q_2(\{K_k,A_k\})T_\lambda d\lambda + \int_0^1 T_\lambda^*E_{Q_1}(K_k,A_k))T_\lambda d\lambda \tag{56}$$

Lemma 2.9 (Action of T_λ on quadratic operators)**.**

$$T_\lambda^*Q_1(A_K)T_\lambda = Q_1(A_k) + \int_0^\lambda T_{\lambda'}^*(Q_2(\{K_k,A_k\})T_{\lambda'}d\lambda' + \int_0^\lambda T_{\lambda'}^*E_{Q_1}(K_k,A_k))T_{\lambda'}d\lambda' \tag{57}$$

$$T_\lambda^*Q_2(A_K)T_\lambda = Q_2(A_k) + \int_0^\lambda T_{\lambda'}^*(Q_1(\{K_k,A_k\})T_{\lambda'}d\lambda' + \int_0^\lambda T_{\lambda'}^*E_{Q_2}(K_k,A_k))T_{\lambda'}d\lambda' \tag{58}$$
$$+ \int_0^\lambda T_{\lambda'}^*\epsilon(\ell)T_{\lambda'}d\lambda' \tag{59}$$

Proof. We prove the above by using the Duhamel's formula, redoing the above computation (53) through (56). □

Proposition 2.10 (Action of T_1 on $Q_2(A_k)$)**.**

$$T_1^* Q_2(A_K) T_1 = Q_2\left(\sum_{m\geq 0} \frac{\Theta_K^{2m}(A_k)}{(2m)!}\right) + Q_1\left(\sum_{m\geq 0} \frac{\Theta_K^{2m+1}(A_k)}{(2m+1)!}\right)$$

$$+ \int_0^1 \int_0^\lambda \dots \int_0^{\lambda_{n-1}} T_{\lambda_n}^* (Q_{\sigma(n)}(\Theta_K^n(A_k)) T_{\lambda_n} d\lambda_n \dots d\lambda_1 d\lambda \tag{60}$$

$$+ \sum_{n\geq 0} \int_0^\lambda \int_0^{\lambda_1} \cdots \int_0^{\lambda_2 n+1} T_\lambda^* \Theta_K^n(\epsilon(\ell)) T_\lambda d\lambda d\lambda_1 \dots d\lambda_{2n+1} + \sum_{i=1}^n E_i \tag{61}$$

where $\sigma(n) = \begin{cases} 1 & \textit{for } n \textit{ even} \\ 2 & \textit{for } n \textit{ odd.} \end{cases}$.

Proof. We have, from (56),

$$T_1^* Q_1(A_K) T_1 = Q_1(A_k) + \int_0^1 T_\lambda^* (Q_2(\{K_k, A_k\}) T_\lambda d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k)) T_\lambda d\lambda \tag{62}$$

We use (59) from Lemma 2.9 above to arrive at

$$(62) = Q_1(A_k) + \frac{1}{1!} Q_2(\{K_k, A_k\}) + \int_0^1 \int_0^\lambda T_{\lambda_1}^* (Q_1(\{K_k, \{K_k, A_k\}\}) T_{\lambda_1} d\lambda_1 d\lambda$$

$$+ \int_0^1 \int_0^\lambda T_{\lambda_1}^* (E_{Q_2}(K_k, \{K_k, A_k\}) T_{\lambda_1} d\lambda_1 d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k)) T_\lambda d\lambda. \tag{63}$$

Next we use (57) from Lemma 2.9

$$(63) = Q_1(A_k) + \frac{1}{1!} Q_2(\{K_k, A_k\}) + \frac{1}{2!} Q_1(\{K_k, \{K_k, A_k\}\})$$

$$+ \int_0^1 \int_0^\lambda \int_0^{\lambda_1} T_{\lambda_2}^* (Q_2(\{K_k, \{K_k, \{K_k, A_k\}\}\}) T_{\lambda_2} d\lambda_2 d\lambda_1 d\lambda$$

$$+ \int_0^1 \int_0^\lambda \int_0^{\lambda_1} T_{\lambda_2}^* E_{Q_1}(K_k, \{K_k, \{K_k, A_k\}\}) T_{\lambda_2} d\lambda_2 d\lambda_1 d\lambda$$

$$+ \int_0^1 \int_0^\lambda T_{\lambda_1}^* E_{Q_2}(K_k, \{K_k, A_k\}) T_{\lambda_1} d\lambda_1 d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k) T_\lambda d\lambda. \tag{64}$$

For our convenience, we introduce the following notation for writing the nested anti-commutators

$$\Theta_K^n(A(\ell)) = \underbrace{\{K(\ell), \{\dots, \{K(\ell)}_{\text{n times}}, A(\ell)\} \dots\}\} \tag{65}$$

with

$$\Theta_K^0(A_k) = A_k. \tag{66}$$

We also introduce another notation for the error terms

$$E_n(K(\ell), A(\ell)) = \begin{cases} \int\limits_{\Delta^{2n}} T_\lambda^* E_{Q_1}\left(\Theta_K^{2n}(A(\ell)), K(\ell)\right) T_\lambda d\lambda & \text{for n even} \\ \int\limits_{\Delta^{2n-1}} T_\lambda^* E_{Q_2}\left(\Theta_K^{2n-1}(A(\ell)), K(\ell)\right) T_\lambda d\lambda & \text{for n odd} \end{cases}. \tag{67}$$

Then after multiple interations we arrive at

$$\begin{aligned} T_1^* Q_1(A_K) T_1 &= Q_1(\Theta_K^0(A_k)) + \frac{1}{1!} Q_2(\Theta_K^1(A_k)) + \frac{1}{2!} Q_1(\Theta_K^2(A_k)) \\ &+ \frac{1}{3!} Q_1(\Theta_K^3(A_k)) + \dots \\ &+ \int_0^1 \int_0^\lambda \dots \int_0^{\lambda_{n-1}} T_{\lambda_n}^* (Q_{\sigma(n)}(\Theta_K^n(A_k)) T_{\lambda_n} d\lambda_n \dots d\lambda_1 d\lambda \\ &+ E_n(K_k, A_k) + E_{n-1}(K_k, A_k) + \dots + E_1(K_k, A_k) \qquad (68) \\ &= Q_1 \left(\sum_{m \geq 0} \frac{\Theta_K^{2m}(A_k)}{(2m)!} \right) + Q_2 \left(\sum_{m \geq 0} \frac{\Theta_K^{2m+1}(A_k)}{(2m+1)!} \right) \\ &+ \int_0^1 \int_0^\lambda \dots \int_0^{\lambda_{n-1}} T_{\lambda_n}^* (Q_{\sigma(n)}(\Theta_K^n(A_k)) T_{\lambda_n} d\lambda_n \dots d\lambda_1 d\lambda + \sum_{i=1}^n E_i(K_k, A_k) \end{aligned} \tag{69}$$

where $\sigma(n) = \begin{cases} 1 & \text{for n even} \\ 2 & \text{for n odd.} \end{cases}$. □

Proposition 2.11 (Final Expansion). *Change A_K by Δ*

$$\begin{aligned} \langle \Omega, T_1^* \left(n_q + n_{-q}\right) T_1 \Omega \rangle = \Bigg\langle \Omega, \Bigg(& Q_2 \left(\sum_{m \geq 0} \frac{\Theta_K^{2m}(A_k)}{(2m)!} \right) + Q_1 \left(\sum_{m \geq 0} \frac{\Theta_K^{2m+1}(A_k)}{(2m+1)!} \right) \\ &+ \int_0^1 \int_0^\lambda \dots \int_0^{\lambda_{n-1}} T_{\lambda_n}^* (Q_{\sigma(n)}(\Theta_K^n(A_k)) T_{\lambda_n} d\lambda_n \dots d\lambda_1 d\lambda \qquad (70) \\ &+ \sum_{n \geq 0} \int_0^\lambda \int_0^{\lambda_1} \dots \int_0^{\lambda_{2n+1}} T_\lambda^* \Theta_K^n(\epsilon(\ell)) T_\lambda d\lambda d\lambda_1 \dots d\lambda_{2n+1} + \sum_{i=1}^n E_i \Bigg) \Omega \Bigg\rangle \end{aligned} \tag{71}$$

3 Error bounds

Definition 3.1.

$$\Xi_\lambda(k) := \langle T_\lambda \Omega, a_k^* a_k T_\lambda \Omega \rangle \tag{72}$$

$$\Xi_\lambda := \sup_k \langle T_\lambda \Omega, a_k^* a_k T_\lambda \Omega \rangle \tag{73}$$

Lemma 3.2.

$$\langle T_\lambda \Omega, E_n(K_k, A_k) T_\lambda \Omega \rangle \leq e^{||k||} \Xi_\lambda \tag{74}$$

References