Occupation Density

Abstract

The

Keywords: keyword1, Keyword2, Keyword3, Keyword4

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 $L_a^2(\mathbb{T}^{3N}) = \bigwedge_{i=1}^{N} L_a^2(\mathbb{T}^3)$. 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 $\langle \Psi_{trial}, a_l^* a_l \Psi_{trial} \rangle$, $l \in \mathbb{Z}^3$. 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

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

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

We define the pair operators asWrite proper definition of the pair operators

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

for $p \in L_k$

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

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

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

Proof.

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

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

Also, we have the following identity

$$[b_p^*(k), b_q(\ell)] = -[b_p(k), b_q^*(\ell)]^* \tag{13}$$

with the effect of the complex conjugate seen only on the error term as above.

Before we move on, we write some important commutation relations in order to facilitate further computations.

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

$$\left[n_q, a_p^*\right] = \delta_{q.p}a_p^* \tag{14}$$
$$\left[n_q, a_p\right] = -\delta_{q.p}a_p \tag{15}$$

Proof.

$$\begin{aligned}
\left[n_q, a_p^*\right] &= \left[a_q^* a_q, a_p^*\right] \\
&= a_q^* a_q a_p^* - a_p^* a_q^* a_q \\
&= a_q^* \delta_{qp} - a_q^* a_p^* a_q - a_p^* a_q^* a_q \\
&= \delta_{q,p}a_p^*
\end{aligned} \tag{16}$$

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

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

Hence the commutation relation holds □

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

$$\left[n_q, b_p^*(k)\right] = (\delta_{q.p} + \delta_{q.p-k})\, b_p^*(k) \tag{18}$$

$$[n_q, b_p(k)] = -(\delta_{q.p} + \delta_{q.p-k})\, b_p(k). \tag{19}$$

Proof. We begin with the first commutation relation

$$\begin{aligned}
[n_q, b_p^*(k)] &= [n_q, a_p^* a_{p-k}^*] && (20)\\
&= [n_q, a_p^*] a_{p-k}^* + a_p^* [n_q, a_{p-k}^*] && (21)\\
&= \big(\delta_{q,p} + \delta_{q,p-k}\big) b_p^*(k). && (22)
\end{aligned}$$

It follows from the above Lemma 2.2. Similarly we observe

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

And we attain the said relation for the second commutator. □

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

$$\mathcal{K} = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \left(b_r(\ell) b_{-s}(-\ell) - b_{-s}^*(-\ell) b_r^*(\ell)\right) \tag{24}$$

Next, we define the Bogoliubov transformation $T = e^{\mathcal{K}}$ which is a unitary due the fact that $\mathcal{K}$ is anti-unitary i.e. $\mathcal{K} = -\mathcal{K}^*$.
Lemma 2.4 (Commutator between $\mathcal{K}$ and pair operators)**.**

$$[b_p^*(k), \mathcal{K}] = -\sum_{s \in L_k} K(k)_{p,s} b_{-s}(-k) + \mathcal{E}_p(k) \tag{25}$$

$$[b_p(k), \mathcal{K}] = -\sum_{s \in L_k} K(k)_{p,s} b_{-s}^*(-k) + (\mathcal{E}_p(k))^* , \tag{26}$$

where,

$$\mathcal{E}_p(k) = -\frac{1}{2} \sum_{l \in \mathbb{Z}_*^3} \sum_{r,s \in L_l} K(\ell)_{r,s} \left\{b_{-s}(-\ell), \epsilon_{r,p}(\ell, l)\right\} \tag{27}$$

Proof. We start with the first commutation relation.

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

$$
\begin{aligned}
&= \frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\Big(\big(-\delta_{p,r}\delta_{k,\ell}-\epsilon_{r,p}(\ell,k)\big)b_{-s}(-\ell)+b_r(\ell)\big(-\delta_{p,-s}\delta_{k,-\ell}-\epsilon_{-s,p}(-\ell,k)\big)\Big)\\
&= -\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(\delta_{p,r}\delta_{k,\ell}\big)b_{-s}(-\ell)-\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(\epsilon_{r,p}(\ell,k)b_{-s}(-\ell)\big)\\
&\quad -\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}b_r(\ell)\big(\delta_{p,-s}\delta_{k,-\ell}\big)-\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(b_r(\ell)\epsilon_{-s,p}(-\ell,k)\big)\\
&= -\frac{1}{2}\sum_{s\in L_k} K(k)_{p,s}b_{-s}(-k)-\frac{1}{2}\sum_{r\in L_{-k}} K(-k)_{r,-p}b_r(-k)\\
&\quad -\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(\epsilon_{r,p}(\ell,k)b_{-s}(-\ell)\big)-\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(b_r(\ell)\epsilon_{-s,p}(-\ell,k)\big).
\end{aligned}
\tag{28}
$$

Consider the second summand, we know that $L_{-k}=-L_k$, then we identify r with $-s$ and we have

$$
-\frac{1}{2}\sum_{-s\in -L_k} K(-k)_{-s,-p}b_{-s}(-k)=-\frac{1}{2}\sum_{s\in L_k} K(k)_{s,p}b_{-s}(-k). \tag{29}
$$

Now, consider the fourth summand, first we exchange r and s and arrive at

$$
-\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(b_s(\ell)\epsilon_{-r,p}(-\ell,k)\big). \tag{30}
$$

Second, we reflect all the summed over momenta (i.e. $\ell\to-\ell, r\to -r, s\to -s$) which provides us

$$
(30) = -\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(b_{-s}(-\ell)\epsilon_{r,p}(\ell,k)\big). \tag{31}
$$

Then substituting (29) and (31) in (28), we get

$$
(28) = -\sum_{s\in L_k} K(k)_{p,s}b_{-s}(-k) \tag{32}
$$

$$
-\frac{1}{2}\sum_{\ell\in\mathbb{Z}^3_*}\sum_{r,s\in L_\ell} K(\ell)_{r,s}\big(\epsilon_{r,p}(\ell,k)b_{-s}(-\ell)+b_{-s}(-\ell)\epsilon_{r,p}(\ell,k)\big) \tag{33}
$$

Here, we observe (33) $=\mathcal{E}_p(k)$. □

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

$$
\mathfrak{R}: a^*_{k_1}\dots a^*_{k_n}\Omega \mapsto a^*_{-k_1}\dots a^*_{-k_n}\Omega \tag{34}
$$

while leaving the vacuum state invariant.

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

$$
\mathfrak{R}T\Omega = T\Omega \tag{35}
$$

Proof. to be filled in □

Next we define the quadratic operator as

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

$$Q_1(A(\ell)) \coloneqq \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} A(\ell)_{r,s} \left(b^*_r(\ell) b_s(\ell) + b^*_s(\ell) b_r(\ell)\right) \tag{36}$$

$$Q_2(A(\ell)) \coloneqq \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} A(\ell)_{r,s} \left(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell)\right) \tag{37}$$

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 $-q$, $(\Delta^q)_{m,s} \coloneqq -\frac{1}{2}(\delta_{m,q}\delta_{m,s} + \delta_{m,-q}\delta_{m.s})$ and we get*

$$\left\langle \Omega, T_1^* \frac{1}{2} \left(n_q + n_{-q}\right) T_1 \Omega \right\rangle = \frac{1}{2} \int_0^1 d\lambda \left\langle \Omega, T_\lambda^* Q_2 \Big(\left\{ K(\ell), \Delta^q \right\} \Big) T_\lambda \Omega \right\rangle \tag{38}$$

Proof. We start by applying Duhamel's formula to RHS of (38) and we have

$$\frac{1}{2} \left(\langle \Omega, \left(n_q + n_{-q}\right) \Omega \rangle + \int_0^1 d\lambda \left(\frac{d}{d\lambda} \langle \Omega, T_\lambda^* \left(n_q + n_{-q}\right) T_\lambda \Omega \rangle \right) \right) \tag{39}$$

$$= \frac{1}{2} \int_0^1 d\lambda \left(\langle \Omega, T_\lambda^* (-\mathcal{K}) \left(n_q + n_{-q}\right) T_\lambda + T_\lambda^* \left(n_q + n_{-q}\right) (\mathcal{K}) T_\lambda \Omega \rangle \right) \tag{40}$$

$$= \frac{1}{2} \int_0^1 d\lambda \, \langle \Omega, T_\lambda^* [\left(n_q + n_{-q}\right), \mathcal{K}] T_\lambda \Omega \rangle \, . \tag{41}$$

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

$$[n_q, \mathcal{K}] = \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \left[a^*_q a_q, \left(b_r(\ell) b_{-s}(-\ell) - b^*_{-s}(-\ell) b^*_r(\ell) \right) \right] \tag{42}$$

$$= \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Bigg(\left[a^*_q a_q, b_r(\ell) \right] b_{-s}(-\ell) + b_r(\ell) \left[a^*_q a_q, b_{-s}(-\ell) \right] \tag{43}$$

$$- \left[a^*_q a_q, b^*_{-s}(-\ell) \right] b^*_r(\ell) - b^*_{-s}(-\ell) \left[a^*_q a_q, b^*_r(\ell) \right] \Bigg) \tag{44}$$

$$= \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Bigg((-1) \left(\delta_{q.r} + \delta_{q.r-\ell} + \delta_{q,-s} + \delta_{q,-s+\ell} \right) \tag{45}$$

$$\times \left(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \right) \Bigg) \tag{46}$$

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

$$[n_q, \mathcal{K}] = \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big((-1)(\delta_{q.r} + \delta_{q,-s}) \big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big). \tag{47}$$

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

$$[n_{-q}, \mathcal{K}] = \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big((-1)(\delta_{-q.r} + \delta_{-q,-s}) \big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big). \tag{48}$$

Next we substitute commutators (47) and (48) in (41),

$$\begin{aligned}
(41) = \frac{1}{2} \int_0^1 d\lambda \Big\langle \Omega, T^*_\lambda \Big(\frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \Big((-1)(\delta_{q.r} + \delta_{q,-s} + \delta_{-q.r} + \delta_{-q,-s}) \\
\times \big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big) \Big) T_\lambda \Omega \Big\rangle \\
= \frac{1}{2} \int_0^1 d\lambda \Big\langle \Omega, T^*_\lambda \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} (-\frac{1}{2}) \Big(\underbrace{K(\ell)_{r,s} (\delta_{q.r} + \delta_{q,-s} + \delta_{-q.r} + \delta_{-q,-s})}_{\text{interpret as matrix product}} \\
\times \big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{49}$$

$$\begin{aligned}
= \frac{1}{2} \int_0^1 d\lambda \Big\langle \Omega, T^*_\lambda \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big(K(\ell)_{r,m} (-\frac{1}{2}) \underbrace{(\delta_{m,q} \delta_{m,s} + \delta_{m,-q} \delta_{m.s})}_{\text{(a)}} \\
+ (-\frac{1}{2}) \underbrace{(\delta_{r,q} \delta_{r,m} + \delta_{r,-q} \delta_{r.m})}_{\text{(b)}} K(\ell)_{m,s} \Big) \big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{50}$$

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

$$\begin{aligned}
(50) = \frac{1}{2} \int_0^1 d\lambda \Big\langle \Omega, T^*_\lambda \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big(K(\ell)_{r,m} \Delta^q_{m,s} + \Delta^q_{r,m} K(\ell)_{m,s} \Big) \\
\big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{51}$$

$$\begin{aligned}
= \frac{1}{2} \int_0^1 d\lambda \Big\langle \Omega, T^*_\lambda \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big(K(\ell)_{r,m} \Delta^q_{m,s} + \Delta^q_{r,m} K(\ell)_{m,s} \Big) \\
\big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big) T_\lambda \Omega \Big\rangle
\end{aligned} \tag{52}$$

$$= \frac{1}{2} \int_0^1 d\lambda \Big\langle \Omega, T^*_\lambda \Big(\sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} \Big\{ K(\ell), \Delta^q \Big\}_{r,s} \big(b_r(\ell) b_{-s}(-\ell) + b^*_{-s}(-\ell) b^*_r(\ell) \big) \Big) T_\lambda \Omega \Big\rangle \tag{53}$$

Using the definition of Q_2, (37), we arrive at

$$(53) = \frac{1}{2}\int_0^1 d\lambda \Big\langle \Omega, T_\lambda^* Q_2\Big(\big\{K(\ell), \Delta^q\big\}\Big) T_\lambda \Omega \Big\rangle \tag{54}$$

□

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

$$[Q_1(A(\ell)), \mathcal{K}] = Q_2(\{K(\ell), A(\ell)\}) + E_{Q_1}(A(\ell)) \tag{55}$$
$$[Q_2(B(\ell)), \mathcal{K}] = Q_1(\{K(\ell), B(\ell)\}) + E_{Q_2}(B(\ell)) \tag{56}$$

where,

$$E_{Q_1}(A(\ell)) = -\left(b_r(\ell)\mathcal{E}^*_{-s}(-\ell) + \mathcal{E}_r(\ell)b_{-s}(\ell) + \mathcal{E}_{-s}(-\ell)b^*_r(\ell) + b^*_{-s}(-\ell)\mathcal{E}^*_r(\ell)\right) \tag{57}$$
$$E_{Q_2}(B(\ell)) = -\left(b^*_r(\ell)\mathcal{E}^*_{-s}(-\ell) + \mathcal{E}_r(\ell)b_{-s}(\ell) + \mathcal{E}_{-s}(-\ell)b_r(\ell) + b^*_{-s}(-\ell)\mathcal{E}^*_r(\ell)\right) \tag{58}$$

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

$$\begin{aligned}
[Q_2(B_k), \mathcal{K}] &= \left[\mathcal{K}, \sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q\in L_k} B(k)_{p,q}\left(b^*_p(k)b^*_q(k) + b_p(k)b_q(k)\right)\right] \\
&= \sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q\in L_k} B(k)_{p,q}\left[\mathcal{K}, \left(b^*_p(k)b^*_q(k) + b_p(k)b_q(k)\right)\right] \\
&= \sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q\in L_k} B(k)_{p,q}\left([\mathcal{K}, b^*_p(k)b^*_q(k)] + [\mathcal{K}, b_p(k)b_q(k)]\right) \\
&= \sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q\in L_k} B(k)_{p,q}\left([\mathcal{K}, b^*_p(k)]b^*_q(k) + b^*_p(k)[\mathcal{K}, b^*_q(k)]\right. \\
&\quad \left. + [\mathcal{K}, b_p(k)]b_q(k) + b_p(k)[\mathcal{K}, b_q(k)]\right)
\end{aligned} \tag{59}$$

Now we use the commutation relation from (25) and (26) to get

$$\begin{aligned}
&\sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q\in L_k} B(k)_{p,q}\left(\left(\sum_{r\in L_k} K(k)_{p,r}b_{-r}(-k) + \mathcal{E}_p(k)\right)b^*_q(k) + b^*_p(k)\left(\sum_{r\in L_k} K(k)_{q,r}b_{-r}(-k) + \mathcal{E}_q(k)\right)\right. \\
&+ \left.\left(\sum_{r\in L_k} K(k)_{r,p}b^*_{-r}(-k) + \mathcal{E}^*_p(k)\right)b_q(k) + b_p(k)\left(\sum_{r\in L_k} K(k)_{r,q}b^*_{-r}(-k) + \mathcal{E}^*_q(k)\right)\right) \\
&= \sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q,r\in L_k} B(k)_{p,q}\left(K(k)_{p,r}b_{-r}(-k)b^*_q(k) + b^*_p(k)K(k)_{q,r}b_{-r}(-k)\right. \\
&\qquad\qquad \left. + K(k)_{r,p}b^*_{-r}(-k)b_q(k) + b_p(k)K(k)_{r,q}b^*_{-r}(-k)\right) \\
&+ \sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q\in L_k} B(k)_{p,q}\left(\mathcal{E}_p(k)b^*_q(k) + b^*_p(k)\mathcal{E}_q(k) + b_p(k)\mathcal{E}^*_q(k) + \mathcal{E}^*_p(k)b_q(k)\right).
\end{aligned} \tag{60}$$

Nest, we denote the second sum term as the error: $E_{Q_2}(B_k)$ and we arrive at

$$\sum_{\ell\in\mathbb{Z}^3_*}\sum_{p,q,r\in L_k} B(k)_{p,q}\left(K(k)_{p,r}b_{-r}(-k)b^*_q(k) \;+\; b^*_p(k)K(k)_{q,r}b_r(k)\right.$$

$$+ K(k)_{r,p} b_r^*(k) b_q(k) + b_p(k) K(k)_{r,q} b_r^*(k)) + E_{Q_2}(B_k). \quad (61)$$

Next we remove the duplicate index and write it in a condensed way

$$\sum_{\ell \in \mathbb{Z}^3_*} \sum_{p,q,r \in L_k} B(k)_{p,q} \left(K(k)_{p,r} b_r(k) b_q^*(k) + b_p^*(k) K(k)_{q,r} b_r(k) \right.$$

$$\left. + K(k)_{r,p} b_r^*(k) b_q(k) + b_p(k) K(k)_{r,q} b_r^*(k) \right) + E_{Q_2}(B_k) \quad (62)$$

$$= \sum_{\ell \in \mathbb{Z}^3_*} \sum_{p,q \in L_k} \left(\{K_k, B_k\}_{p,q} b_p(k) b_q^*(k) + \{K_k, B_k\}_{p,q} b_p^*(k) b_q(k) \right) + E_{Q_2}(B_k) \quad (63)$$

$$= \sum_{\ell \in \mathbb{Z}^3_*} \sum_{p,q \in L_k} \{K_k, B_k\}_{p,q} \left(b_p(k) b_q^*(k) + b_p^*(k) b_q(k) \right) + E_{Q_2}(B_k) \quad (64)$$

$$= Q_1(\{K_k, B_k\}) + E_{Q_2}(B_k). \quad (65)$$

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

2.1 Transformation of quadratic operators

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

$$T_1^* Q_1(A(\ell))T_1 = Q_1(A(\ell)) + \int_0^1 \frac{d}{d\lambda}\left(T_\lambda^* Q_1(A(\ell))T_\lambda\right) d\lambda \tag{66}$$

$$= Q_1(A_k) + \int_0^1 T_\lambda^* [\mathcal{K}, Q_1(A_k)] T_\lambda d\lambda. \tag{67}$$

Then from the lemma above, we get

$$(67) = Q_1(A_k) + \int_0^1 T_\lambda^* (Q_2(\{K_k, A_k\}) + E_{Q_1}(K_k, A_k))T_\lambda d\lambda \tag{68}$$

$$= Q_1(A_k) + \int_0^1 T_\lambda^* (Q_2(\{K_k, A_k\})T_\lambda d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k))T_\lambda d\lambda \tag{69}$$

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

$$T_\lambda^* Q_1(A_K)T_\lambda = Q_1(A_k) + \int_0^\lambda T_{\lambda'}^* (Q_2(\{K_k, A_k\})T_{\lambda'} d\lambda' + \int_0^\lambda T_{\lambda'}^* E_{Q_1}(K_k, A_k))T_{\lambda'} d\lambda' \tag{70}$$

$$T_\lambda^* Q_2(A_K)T_\lambda = Q_2(A_k) + \int_0^\lambda T_{\lambda'}^* (Q_1(\{K_k, A_k\})T_{\lambda'} d\lambda' + \int_0^\lambda T_{\lambda'}^* E_{Q_2}(K_k, A_k))T_{\lambda'} d\lambda' \tag{71}$$

$$+ \int_0^\lambda T_{\lambda'}^* \epsilon(\ell) T_{\lambda'} d\lambda' \tag{72}$$

Proof. We prove the above by using the Duhamel's formula, redoing the above computation (66) through (69). □

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

$$T_1^* Q_2(A_K)T_1 = Q_2\left(\sum_{m\geq 0} \frac{\Theta_K^{2m}(A_k)}{(2m)!}\right) + Q_1\left(\sum_{m\geq 0} \frac{\Theta_K^{2m+1}(A_k)}{(2m+1)!}\right)$$
$$+ \int_0^1 \int_0^\lambda \dots \int_0^{\lambda_{n-1}} T_{\lambda_n}^* (Q_{\sigma(n)}(\Theta_K^n(A_k))T_{\lambda_n} d\lambda_n \dots d\lambda_1 d\lambda \tag{73}$$

$$+ \sum_{n\geq 0} \int_0^\lambda \int_0^{\lambda_1} \cdots \int_0^{\lambda_2 n+1} T_\lambda^* \Theta_K^n(\epsilon(\ell)) T_\lambda d\lambda d\lambda_1 \dots d\lambda_{2n+1} + \sum_{i=1}^n E_i \tag{74}$$

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

Proof. We have, from (69),

$$T_1^* Q_1(A_K)T_1 = Q_1(A_k) + \int_0^1 T_\lambda^*(Q_2(\{K_k, A_k\})T_\lambda d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k))T_\lambda d\lambda \quad (75)$$

We use (72) from Lemma 2.9 above to arrive at

$$\begin{aligned}(75) = Q_1(A_k) + \frac{1}{1!}Q_2(\{K_k, A_k\}) + \int_0^1\int_0^\lambda T_{\lambda_1}^*(Q_1(\{K_k, \{K_k, A_k\}\})T_{\lambda_1} d\lambda_1 d\lambda \\ + \int_0^1\int_0^\lambda T_{\lambda_1}^*(E_{Q_2}(K_k, \{K_k, A_k\})T_{\lambda_1} d\lambda_1 d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k))T_\lambda d\lambda. \quad (76)\end{aligned}$$

Next we use (70) from Lemma 2.9

$$\begin{aligned}(76) &= Q_1(A_k) + \frac{1}{1!}Q_2(\{K_k, A_k\}) + \frac{1}{2!}Q_1(\{K_k, \{K_k, A_k\}\}) \\ &+ \int_0^1\int_0^\lambda\int_0^{\lambda_1} T_{\lambda_2}^*(Q_2(\{K_k, \{K_k, \{K_k, A_k\}\}\})T_{\lambda_2} d\lambda_2 d\lambda_1 d\lambda \\ &+ \int_0^1\int_0^\lambda\int_0^{\lambda_1} T_{\lambda_2}^* E_{Q_1}(K_k, \{K_k, \{K_k, A_k\}\})T_{\lambda_2} d\lambda_2 d\lambda_1 d\lambda \\ &+ \int_0^1\int_0^\lambda T_{\lambda_1}^* E_{Q_2}(K_k, \{K_k, A_k\})T_{\lambda_1} d\lambda_1 d\lambda + \int_0^1 T_\lambda^* E_{Q_1}(K_k, A_k)T_\lambda d\lambda. \quad (77)\end{aligned}$$

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

$$\Theta_K^n(A(\ell)) = \underbrace{\{K(\ell), \{\ldots, \{K(\ell)}_{\text{n times}}, A(\ell)\}\ldots\}\} \quad (78)$$

with

$$\Theta_K^0(A_k) = A_k. \quad (79)$$

We also introduce another notation for the error terms

$$E_n(K(\ell), A(\ell)) = \begin{cases} \int_{\Delta^{2n}} T_\lambda^* E_{Q_1}\left(\Theta_K^{2n}(A(\ell)), K(\ell)\right) T_\lambda d\lambda & \text{for n even} \\ \int_{\Delta^{2n-1}} T_\lambda^* E_{Q_2}\left(\Theta_K^{2n-1}(A(\ell)), K(\ell)\right) T_\lambda d\lambda & \text{for n odd} \end{cases}. \quad (80)$$

Then after multiple interations we arrive at

$$\begin{aligned}T_1^* Q_1(A_K)T_1 = Q_1(\Theta_K^0(A_k)) + \frac{1}{1!}Q_2(\Theta_K^1(A_k)) + \frac{1}{2!}Q_1(\Theta_K^2(A_k)) \\ + \frac{1}{3!}Q_1(\Theta_K^3(A_k)) + \ldots\end{aligned}$$

$$
\begin{aligned}
&+\int_0^1\int_0^\lambda\dots\int_0^{\lambda_{n-1}} T^*_{\lambda_n}(Q_{\sigma(n)}(\Theta_K^n(A_k))T_{\lambda_n}d\lambda_n\dots d\lambda_1 d\lambda \\
&+E_n(K_k,A_k)+E_{n-1}(K_k,A_k)+\dots+E_1(K_k,A_k) && (81)\\
&=Q_1\left(\sum_{m\geq 0}\frac{\Theta_K^{2m}(A_k)}{(2m)!}\right)+Q_2\left(\sum_{m\geq 0}\frac{\Theta_K^{2m+1}(A_k)}{(2m+1)!}\right)\\
&+\int_0^1\int_0^\lambda\dots\int_0^{\lambda_{n-1}} T^*_{\lambda_n}(Q_{\sigma(n)}(\Theta_K^n(A_k))T_{\lambda_n}d\lambda_n\dots d\lambda_1 d\lambda+\sum_{i=1}^n E_i(K_k,A_k) && (82)
\end{aligned}
$$

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*

$$
\begin{aligned}
\langle\Omega,T_1^*\left(n_q+n_{-q}\right)T_1\Omega\rangle=\Bigg\langle\Omega,\Bigg(&Q_2\left(\sum_{m\geq 0}\frac{\Theta_K^{2m}(A_k)}{(2m)!}\right)+Q_1\left(\sum_{m\geq 0}\frac{\Theta_K^{2m+1}(A_k)}{(2m+1)!}\right)\\
&+\int_0^1\int_0^\lambda\dots\int_0^{\lambda_{n-1}} T^*_{\lambda_n}(Q_{\sigma(n)}(\Theta_K^n(A_k))T_{\lambda_n}d\lambda_n\dots d\lambda_1 d\lambda && (83)\\
&+\sum_{n\geq 0}\int_0^\lambda\int_0^{\lambda_1}\cdots\int_0^{\lambda_2 n+1} T^*_\lambda\Theta_K^n(\epsilon(\ell))T_\lambda d\lambda d\lambda_1\dots d\lambda_{2n+1}+\sum_{i=1}^n E_i\Bigg)\Omega\Bigg\rangle && (84)
\end{aligned}
$$

Proof. to be filled in □

3 Error bounds

Definition 3.1.

$$\Xi_\lambda(k):=\langle T_\lambda\Omega,a_k^*a_kT_\lambda\Omega\rangle \qquad (85)$$

$$\Xi_\lambda:=\sup_k\langle T_\lambda\Omega,a_k^*a_kT_\lambda\Omega\rangle \qquad (86)$$

Lemma 3.2.

$$\langle T_\lambda\Omega,E_n(K_k,A_k)T_\lambda\Omega\rangle\leq e^{||k||}\Xi_\lambda \qquad (87)$$

References