

EM Response for Quartic Hamiltonian (etc.)

1 Current Per Orbital Setup

We revisit the derivation of the expression for current per orbital, making sure that each step carries over for the case of quartic and other more general Hamiltonians.

We take as our starting point an eigenstate of an (e.g.) quartic wavefunction, which may be written as a sum over ordinary Landau level states

$$|\lambda\rangle = \sum_m C_m^\lambda |m\rangle,$$

normalised so that

$$\sum_m |C_m^\lambda|^2 = 1.$$

This eigenstate is associated with some energy E_λ . In contrast to previous calculations, we are not particularly interested in the series of perturbative corrections at $O(B^m)$. These corrections may be straightforwardly incorporated into the coefficients C_m^λ and energy E_λ , but we will not keep track of them order by order.

We are really interested in the EM response of the *band* corresponding to state $|\lambda\rangle$. Assuming the Landau gauge, we write states within the band as $|\lambda, k_x\rangle$, with k_x a linear momentum. We make our usual approximation and assume the bands are completely flat, and ignore any tunnelling and discreteness effects that arise due to the underlying lattice Hamiltonian.

As before, we obtain the current per orbital by first perturbing the orbital state $|\lambda, k_x\rangle$ with an external sinusoidal potential, obtaining

$$|\tilde{\lambda}, k_x\rangle = |\lambda, k_x\rangle + \sum_{\mu \neq \lambda} \frac{\langle \mu, k_x | \hat{V}(x) | \lambda, k_x \rangle}{E_\lambda - E_\mu} |\mu, k_x\rangle.$$

We then calculate the expectation value of the current operator in this perturbed state, giving

$$\langle \hat{I}_y \rangle = \sum_{\mu \neq \lambda} \langle \lambda, k_x | \hat{I}_y | \mu, k_x \rangle \frac{\langle \mu, k_x | \hat{V}(x) | \lambda, k_x \rangle}{E_\lambda - E_\mu}.$$

We now need expressions for $\hat{V}(x)$ and \hat{I}_y . For the former, we use the same sinusoidal potential as before, writing

$$\hat{V}(x) = \sum_p c_p (\hat{x} - x_0)^p = \sum_p c_p (2B)^{p/2} (a + a^\dagger)^p,$$

where c_p can be expressed in terms of q or derivatives of E if required. For the current operator, we take the derivative of the Hamiltonian,

$$\hat{I}_y = ev_y = \partial H / \partial k_y.$$

We therefore require an explicit expression for the Hamiltonian.

Hamiltonian Expressions

For now, we write

$$\hat{H}_{2n} = \alpha_{2n} \hat{k}_x^{2n} + \beta_{2n} \hat{k}_y^{2n},$$

where α_{2n} and β_{2n} are unspecified coefficients. The notation \hat{k}_x and \hat{k}_y is taken from the EM response paper: I think this is as the same as Π_x and Π_y in David's paper.

Let's see if we can obtain standard expressions in terms of ladder operators. We recall that

$$\begin{aligned} a &= \frac{i}{\sqrt{2B}} (\hat{k}_x + i\hat{k}_y) \\ a^\dagger &= \frac{i}{\sqrt{2B}} (-\hat{k}_x + i\hat{k}_y) \end{aligned}$$

so that

$$\begin{aligned} a + a^\dagger &= -\sqrt{\frac{2}{B}} \hat{k}_y \\ a - a^\dagger &= i\sqrt{\frac{2}{B}} \hat{k}_x \end{aligned}$$

and so

$$\begin{aligned} \hat{k}_y &= -\sqrt{\frac{B}{2}} (a + a^\dagger) \\ \hat{k}_x &= -i\sqrt{\frac{B}{2}} (a - a^\dagger). \end{aligned}$$

Substituting in, and actually ignoring the coefficients, we find

$$\hat{H}_{2n} = \left(\frac{B}{2}\right)^n \left[(-1)^n (a - a^\dagger)^{2n} + (a + a^\dagger)^{2n} \right].$$

We write out the first few (where number in brackets refers to powers):

$$\begin{aligned} \hat{H}_{2 \times 1} &= B [2a^\dagger(1)a(1) + 1] \\ \hat{H}_{2 \times 2} &= B^2 \left[6a^\dagger(1)a(1) + 3a^\dagger(2)a(2) + \frac{a(4)}{2} + \frac{a^\dagger(4)}{2} + \frac{3}{2} \right] \\ \hat{H}_{2 \times 3} &= B^3 \left[\frac{45}{2}a^\dagger(1)a(1) + \frac{3}{2}a^\dagger(1)a(5) + \frac{45}{2}a^\dagger(2)a(2) + 5a^\dagger(3)a(3) + \frac{3}{2}a^\dagger(5)a(1) + \frac{15a(4)}{4} + \frac{15a^\dagger(4)}{4} + \frac{15}{4} \right] \\ \hat{H}_{2 \times 4} &= B^4 \left[105a^\dagger(1)a(1) + 21a^\dagger(1)a(5) + \frac{315}{2}a^\dagger(2)a(2) + \frac{7}{2}a^\dagger(2)a(6) + 70a^\dagger(3)a(3) + \frac{35}{4}a^\dagger(4)a(4) \right. \\ &\quad \left. + 21a^\dagger(5)a(1) + \frac{7}{2}a^\dagger(6)a(2) + \frac{105a(4)}{4} + \frac{a(8)}{8} + \frac{105a^\dagger(4)}{4} + \frac{a^\dagger(8)}{8} + \frac{105}{8} \right]. \end{aligned}$$

Checking coefficients (including $\hat{H}_{2 \times 5}$ and $\hat{H}_{2 \times 6}$), the Hamiltonian may be written

$$\begin{aligned} \hat{H}_{2n} &= \frac{(2n-1)!!}{2^{n-1}} B^n \left\{ 1 + (2n) a^\dagger a + n(n-1) (a^\dagger)^2 a^2 + \frac{1}{6} n(n-1) \left[(a^\dagger)^4 + a^4 \right] \right. \\ &\quad + \frac{1}{15} n(n-1)(n-2) \left[(a^\dagger)^5 a + a^\dagger a^5 \right] + \frac{2}{9} n(n-1)(n-2) (a^\dagger)^3 a^3 \\ &\quad + \frac{1}{90} n(n-1)(n-2)(n-3) \left[(a^\dagger)^6 a^2 + (a^\dagger)^2 a^6 \right] + \frac{1}{36} n(n-1)(n-2)(n-3) (a^\dagger)^4 a^4 \\ &\quad \left. + \frac{1}{2520} n(n-1)(n-2)(n-3) \left[(a^\dagger)^8 + a^8 \right] + \dots \right\}, \end{aligned}$$

where this now include all terms present up to $\hat{H}_{2 \times 4}$ (which are also correctly accounted for in higher Hamiltonians).

Let's see if we can also find a general expression for the coefficient of the term of the form $(a^\dagger)^b a^c$. We first look at the diagonal terms for which $a = b$. We find that the general form (except the overall prefactor) may be written

$$\begin{aligned} & \frac{8^b}{(2b)!!(2b)!!} n(n-1) \dots (n-b+1) (a^\dagger)^b a^b \\ &= \frac{2^b}{b!b!} \times \frac{n!}{(n-b)!} (a^\dagger)^b a^b \end{aligned}$$

Using this as motivation, we verify that the *generic* term (again ignoring the prefactor) may be written

$$\frac{2^f}{b!c!} \times \frac{n!}{(n-f)!} (a^\dagger)^b a^c,$$

where

$$f = \frac{b+c}{2}$$

and we sum over all a and b such that $a-b$ is a multiple of four. Overall, we can write

$$\hat{H}_{2n} = \frac{(2n-1)!!n!}{2^{n-1}} B^n \sum_{b,c|(b-c) \in 4\mathbb{Z}} \frac{2^f}{b!c!(n-f)!} (a^\dagger)^b a^c.$$

Finally, we remove the double factorial and simplify to find

$$\hat{H}_{2n} = \frac{(2n)!}{2^{2n-1}} B^n \sum_{b,c|(b-c) \in 4\mathbb{Z}} \frac{2^{\frac{b+c}{2}}}{b!c!(n-(b+c)/2)!} (a^\dagger)^b a^c \quad (1)$$

$$\equiv B^n \sum D_{b,c}^n (a^\dagger)^b a^c. \quad (2)$$

Using Mathematica, we verify that this generates the correct Hamiltonians for $n = 1, 2, 3, 4, 5, 6$.

Current Operator

We are now able to write down an expression for the current operator. We note that

$$\partial_{k_y} a = \partial_{k_y} a^\dagger = -\frac{1}{\sqrt{2B}}$$

and so

$$\hat{I}_y = \partial_{k_y} (\hat{H}_{2n}) = -\frac{B^n}{\sqrt{2B}} \sum D_{b,c}^n \left[b (a^\dagger)^{b-1} a^c + c (a^\dagger)^b a^{c-1} \right].$$

We return to the expected value of the current per orbital,

$$\langle \hat{I}_y \rangle = \sum_{\mu \neq \lambda} \langle \lambda, k_x | \hat{I}_y | \mu, k_x \rangle \frac{\langle \mu, k_x | \hat{V}(x) | \lambda, k_x \rangle}{E_\lambda - E_\mu}.$$

The current operator enters the first factor of each term in the sum. We expand this as

$$\begin{aligned} \langle \lambda, k_x | \hat{I}_y | \mu, k_x \rangle &= \sum_{s,t} C_s^{\lambda*} C_t^\mu \langle s | \left[-\frac{B^n}{\sqrt{2B}} \sum_{b,c} D_{b,c}^n \left[b (a^\dagger)^{b-1} a^c + c (a^\dagger)^b a^{c-1} \right] \right] | t \rangle \\ &= -\frac{B^n}{\sqrt{2B}} \sum_{s,t} \sum_{b,c} D_{b,c}^n C_s^{\lambda*} C_t^\mu \langle s | \left[b (a^\dagger)^{b-1} a^c + c (a^\dagger)^b a^{c-1} \right] | t \rangle. \end{aligned}$$

We now use the relations

$$\begin{aligned}
a^\alpha |m\rangle &= \sqrt{m(m-1)\dots(m-\alpha+1)} |m-\alpha\rangle \\
&= \sqrt{\frac{m!}{(m-\alpha)!}} |m-\alpha\rangle \\
a^{\dagger\alpha} |m\rangle &= \sqrt{(m+1)(m+2)\dots(m+\alpha)} |m+\alpha\rangle \\
&= \sqrt{\frac{(m+\alpha)!}{m!}} |m+\alpha\rangle
\end{aligned}$$

to write

$$\begin{aligned}
c (a^\dagger)^b a^{c-1} |t\rangle &= c (a^\dagger)^b a^{c-1} |t\rangle \\
&= c (a^\dagger)^b \sqrt{\frac{t!}{(t-c+1)!}} |t-c+1\rangle \\
&= c \sqrt{\frac{(t+b-c+1)!}{(t-c+1)!}} \sqrt{\frac{t!}{(t-c+1)!}} |t+b-c+1\rangle
\end{aligned}$$

and

$$b (a^\dagger)^{b-1} a^c |t\rangle = b \sqrt{\frac{(t+b-c-1)!}{(t-c)!}} \sqrt{\frac{t!}{(t-c)!}} |t+b-c-1\rangle$$

so that

$$\begin{aligned}
\langle s | \left[b (a^\dagger)^{b-1} a^c + c (a^\dagger)^b a^{c-1} \right] |t\rangle &= c \sqrt{\frac{(t+b-c+1)!}{(t-c+1)!}} \sqrt{\frac{t!}{(t-c+1)!}} \delta_{s,t+b-c+1} \\
&\quad + b \sqrt{\frac{(t+b-c-1)!}{(t-c)!}} \sqrt{\frac{t!}{(t-c)!}} \delta_{s,t+b-c-1}.
\end{aligned}$$

The first factor finally becomes

$$\begin{aligned}
\langle \lambda, k_x | \hat{I}_y | \mu, k_x \rangle &= -\frac{B^n}{\sqrt{2B}} \sum_{s,t} \sum_{b,c} D_{b,c}^n C_s^{\lambda*} C_t^\mu \left[c \sqrt{\frac{(t+b-c+1)!}{(t-c+1)!}} \sqrt{\frac{t!}{(t-c+1)!}} \delta_{s,t+b-c+1} \right. \\
&\quad \left. + b \sqrt{\frac{(t+b-c-1)!}{(t-c)!}} \sqrt{\frac{t!}{(t-c)!}} \delta_{s,t+b-c-1} \right].
\end{aligned}$$

Let's define another set of coefficients

$$\begin{aligned}
E_{b,c-1}^t &= \sqrt{\frac{(t+b-c+1)!}{(t-c+1)!}} \sqrt{\frac{t!}{(t-c+1)!}} \\
E_{b-1,c}^t &= \sqrt{\frac{(t+b-c-1)!}{(t-c)!}} \sqrt{\frac{t!}{(t-c)!}}
\end{aligned}$$

so that

$$\langle \lambda, k_x | \hat{I}_y | \mu, k_x \rangle = -\frac{B^n}{\sqrt{2B}} \sum_{s,t} \sum_{b,c} D_{b,c}^n C_s^{\lambda*} C_t^\mu \left[c E_{b,c-1}^t \delta_{s,t+b-c+1} + b E_{b-1,c}^t \delta_{s,t+b-c-1} \right]$$

Potential Matrix Elements

We now do a similar calculation for the matrix elements of the periodic potential. We first obtain a general expression for $(a + a^\dagger)^p$. The first few expansions are

$$\begin{aligned}
(a + a^\dagger) &= a(1) + a^\dagger(1) \\
(a + a^\dagger)^2 &= 2a^\dagger(1)a(1) + a(2) + a^\dagger(2) + 1 \\
(a + a^\dagger)^3 &= 3a(1) + a(3) + 3a^\dagger(1) + a^\dagger(3) + 3a^\dagger(1)a(2) + 3a^\dagger(2)a(1) \\
(a + a^\dagger)^4 &= 3a(1) + a(3) + 3a^\dagger(1) + a^\dagger(3) + 3a^\dagger(1)a(2) + 3a^\dagger(2)a(1) \\
(a + a^\dagger)^5 &= 30a^\dagger(1)a(2) + 5a^\dagger(1)a(4) + 30a^\dagger(2)a(1) + 10a^\dagger(2)a(3) + 10a^\dagger(3)a(2) \\
&\quad + 5a^\dagger(4)a(1) + 15a(1) + 10a(3) + a(5) + 15a^\dagger(1) + 10a^\dagger(3) + a^\dagger(5).
\end{aligned}$$

We find a different series for odd versus even p . For odd, we find

$$\begin{aligned}
(a + a^\dagger)^{2q+1} &= (2q+1)!! \left[(a + a^\dagger) + \frac{q}{3} \left((a^\dagger)^3 + a^3 \right) + \frac{q(q-1)}{30} \left((a^\dagger)^5 + a^5 \right) + \frac{q(q-1)(q-2)}{630} \left((a^\dagger)^7 + a^7 \right) \right. \\
&\quad + q \left[(a^\dagger)^2 a + a^\dagger a^2 \right] + \frac{q(q-1)}{6} \left[(a^\dagger)^4 a + a^\dagger a^4 \right] + \frac{q(q-1)}{3} \left[(a^\dagger)^3 a^2 + (a^\dagger)^2 a^3 \right] \\
&\quad + \frac{q(q-1)(q-2)}{18} \left[(a^\dagger)^4 a^3 + (a^\dagger)^3 a^4 \right] + \frac{q(q-1)(q-2)}{30} \left[(a^\dagger)^5 a^2 + (a^\dagger)^2 a^5 \right] + \\
&\quad \left. + \frac{q(q-1)(q-2)}{90} \left[(a^\dagger)^6 a + a^\dagger a^6 \right] \dots \right],
\end{aligned}$$

while for even, we find

$$\begin{aligned}
(a + a^\dagger)^{2q} &= (2q-1)!! \left[1 + q \left((a^\dagger)^2 + a^2 \right) + \frac{q(q-1)}{6} \left((a^\dagger)^4 + a^4 \right) + \frac{q(q-1)(q-2)}{90} \left((a^\dagger)^6 + a^6 \right) \right. \\
&\quad \left. + 2qa^\dagger a + q(q-1) (a^\dagger)^2 a^2 + \frac{2}{3}q(q-1) \left((a^\dagger)^3 a + a^\dagger a^3 \right) + \dots \right].
\end{aligned}$$

We now try to find expressions for the coefficient in front of the term $q(q-1)\dots(a^\dagger)^b a^c$. For the case with just a^\dagger operators (or just a operators), we find for odd $2q+1$ the following sum over odd powers $2j+1$

$$\begin{aligned}
\frac{1}{(2j+1)!!j!} q(q-1)\dots(q-j+1) \left((a^\dagger)^{2j+1} + a^{2j+1} \right) &\equiv \frac{2^{j+1}(j+1)!}{(2j+2)!j!} \frac{q!}{(q-j)!} \left((a^\dagger)^{2j+1} + a^{2j+1} \right) \\
&\equiv \frac{2^{j+1}(j+1)}{(2j+2)!} \frac{q!}{(q-j)!} \left((a^\dagger)^{2j+1} + a^{2j+1} \right) \\
\Rightarrow &= \sum_{b \text{ odd}} \frac{2^{(b+1)/2} \left(\frac{b+1}{2} \right)!}{(b+1)!} \frac{q!}{\left(q - \left(\frac{b-1}{2} \right) \right)!} \left((a^\dagger)^b + a^b \right)
\end{aligned}$$

while we find for even $2q$ we find the sum over even powers $2j$ (including zero):

$$\begin{aligned}
\frac{1}{(2j-1)!!j!} q(q-1)\dots(q-j+1) \left((a^\dagger)^{2j} + a^{2j} \right) &\equiv \frac{2^j}{(2j)!} \frac{q!}{(q-j)!} \left((a^\dagger)^{2j} + a^{2j} \right) \\
\Rightarrow &= \sum_{b \text{ even}} \frac{2^{b/2}}{b!} \frac{q!}{\left(q - \frac{b}{2} \right)!} \left((a^\dagger)^b + a^b \right)
\end{aligned}$$

Let's see if we can find a pattern here...

Odd Terms

Odd terms of the form $(a^\dagger)^b$

We rewrite the above in a more useful form as

$$\frac{1}{b!!((b-1)/2)!} \frac{q!}{\left(q - (b-1)/2 \right)!} (a^\dagger)^b$$

Odd terms of the form $(a^\dagger)^b a$

The pattern is still not very clear, so let's try another subset, this time terms of the form $(a^\dagger)^b a$.

$$\begin{array}{rclcl}
1 & \times & q & \times & (a^\dagger)^2 a \\
\frac{1}{6} & \times & q(q-1) & \times & (a^\dagger)^4 a \\
\frac{1}{90} & \times & q(q-1)(q-2) & \times & (a^\dagger)^6 a \\
\frac{1}{2520} & \times & q(q-1)(q-2)(q-3) & \times & (a^\dagger)^8 a \\
\frac{1}{113400} & \times & q(q-1)(q-2)(q-3)(q-4) & \times & (a^\dagger)^{10} a
\end{array}$$

We see that this is of the form

$$\frac{1}{(b+1-2)!!(b/2)!} \frac{q!}{(q-b/2)!} (a^\dagger)^b a \equiv \frac{1}{(b-1)!!(b/2)!} \frac{q!}{(q-b/2)!} (a^\dagger)^b a.$$

There are a few ways to write this, but we leave it in this form for now...

Odd terms of the form $(a^\dagger)^b a^2$

We do the same for the next set of terms:

$$\begin{array}{rclcl}
\frac{1}{3} & \times & q(q-1) & \times & (a^\dagger)^3 a^2 \\
\frac{1}{30} & \times & q(q-1)(q-2) & \times & (a^\dagger)^5 a^2 \\
\frac{1}{630} & \times & q(q-1)(q-2)(q-3) & \times & (a^\dagger)^7 a^2 \\
\frac{1}{22680} & \times & q(q-1)(q-2)(q-3)(q-4) & \times & (a^\dagger)^9 a^2
\end{array}$$

which we see are of the form

$$\frac{1}{(b)!!((b-1)/2)!} \frac{q!}{(q-(b+1)/2)!} (a^\dagger)^b a^2$$

This is the same as for a^b terms, apart from $b-1 \rightarrow b+1$ in the denominator of the second factor.

Odd terms of the form $(a^\dagger)^b a^3$

We do the same for the next set of terms:

$$\begin{array}{rclcl}
\frac{1}{18} & \times & q(q-1)(q-2) & \times & (a^\dagger)^4 a^3 \\
\frac{1}{270} & \times & q(q-1)(q-2)(q-3) & \times & (a^\dagger)^6 a^3 \\
\frac{1}{7560} & \times & q(q-1)(q-2)(q-3)(q-4) & \times & (a^\dagger)^8 a^3
\end{array}$$

which we see are of the form

$$\frac{1}{3} \frac{1}{(b-1)!!(b/2)!} \frac{q!}{(q-b/2-1)!} (a^\dagger)^b a^3.$$

Odd terms of the form $(a^\dagger)^b a^4$

We do the same for the next set of terms:

$$\begin{array}{rclcl}
\frac{1}{180} & \times & q(q-1)(q-2)(q-3) & \times & (a^\dagger)^5 a^4 \\
\frac{1}{3780} & \times & q(q-1)(q-2)(q-3)(q-4) & \times & (a^\dagger)^7 a^4 \\
\frac{1}{136080} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5) & \times & (a^\dagger)^9 a^4
\end{array}$$

which we see are of the form

$$\frac{1}{6} \frac{1}{(b)!!((b-1)/2)!} \frac{q!}{(q-(b+3)/2)!} (a^\dagger)^b a^4$$

Odd terms of the form $(a^\dagger)^b a^5$

We do the same for the next set of terms:

$$\begin{array}{llll} \frac{1}{2700} & \times & q(q-1)(q-2)(q-3)(q-4) & \times (a^\dagger)^6 a^5 \\ \frac{1}{75600} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5) & \times (a^\dagger)^8 a^5 \\ \frac{1}{3402000} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5)(q-6) & \times (a^\dagger)^{10} a^5 \end{array}$$

which we see are of the form

$$\frac{1}{30} \frac{1}{(b-1)!!(b/2)!} \frac{q!}{(q-b/2-2)!} (a^\dagger)^b a^5.$$

Odd terms of the form $(a^\dagger)^b a^6$

We do the same for the next set of terms:

$$\begin{array}{llll} \frac{1}{56700} & \times & q(q-1)(q-2)(q-3)(q-4) & \times (a^\dagger)^7 a^6 \\ \frac{1}{2041200} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5) & \times (a^\dagger)^9 a^6 \\ \frac{1}{112266000} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5)(q-6) & \times (a^\dagger)^{11} a^6 \end{array}$$

which we see are of the form

$$\frac{1}{90} \frac{1}{(b)!!((b-1)/2)!} \frac{q!}{(q-(b+3)/2)!} (a^\dagger)^b a^4$$

Odd terms of the form $(a^\dagger)^b a^7$

We do the same for the next set of terms:

$$\begin{array}{llll} \frac{1}{1587600} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5)(q-6) & \times (a^\dagger)^8 a^7 \\ \frac{1}{71442000} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5)(q-6)(q-7) & \times (a^\dagger)^{10} a^7 \\ \frac{1}{4715172000} & \times & q(q-1)(q-2)(q-3)(q-4)(q-5)(q-6)(q-7)(q-8) & \times (a^\dagger)^{12} a^7 \end{array}$$

which we see are of the form

$$\frac{1}{630} \frac{1}{(b-1)!!(b/2)!} \frac{q!}{(q-b/2-2)!} (a^\dagger)^b a^7.$$

Odd terms of the form $(a^\dagger)^b a^c$

Since the expressions must be symmetric in b and c , we see that overall the series is a sum of terms

$$(2q+1)!! \sum_{b,c|(b+c) \in 2\mathbb{Z}+1} F_b F_c \frac{q!}{\left(q + \frac{1}{2} - \frac{(b+c)}{2}\right)!} (a^\dagger)^b a^c$$

where $b+c$ is odd, and where F takes different forms depending on the parity of its argument:

$$F_b = \begin{cases} \frac{1}{(b-1)!!(b/2)!} & = \frac{2^{b/2}}{b!} & b \text{ even} \\ \frac{1}{(b)!!((b-1)/2)!} & = \frac{2^{(b-1)/2}}{b!} & b \text{ odd} \end{cases}$$

We can write this more compactly as

$$F_b = \frac{1}{b!} 2^{(b-s_b)/2}$$

where

$$s_b = \frac{1 - (-1)^b}{2} = \begin{cases} 0 & b \text{ even} \\ 1 & b \text{ odd} \end{cases}$$

gives a measure of the parity. The sum should run over all positive b and c with $(b+c) < (2q+1) = p$.

Finally, we try to combine with the initial factor, remove the q dependence and write it in term of p . We note that

$$(2q+1)!! \equiv \frac{(2q+2)!}{2^{q+1}(q+1)!} \equiv (2q+1) \frac{(2q)!}{2^q q!} \equiv \frac{(2q+1)!}{2^q q!}$$

and so

$$\begin{aligned} (2q+1)!! F_b F_c \frac{q!}{\left(q + \frac{1}{2} - \frac{(b+c)}{2}\right)!} (a^\dagger)^b a^c &= F_b F_c \frac{(2q+1)!}{2^q q!} \frac{q!}{\left(q + \frac{1}{2} - \frac{(b+c)}{2}\right)!} (a^\dagger)^b a^c \\ &= \frac{2^{(b+c-s_b-s_c)/2}}{b!c!2^q} \frac{(2q+1)!}{\left(q + \frac{1}{2} - \frac{(b+c)}{2}\right)!} (a^\dagger)^b a^c. \end{aligned}$$

We now replace $q = (p-1)/2$ and note that since $b+c$ is odd, exactly one of s_b and s_c is one, and so

$$\begin{aligned} &= \frac{2^{(b+c-1)/2}}{b!c!2^{(p-1)/2}} \frac{p!}{\left(\frac{p}{2} - \frac{(b+c)}{2}\right)!} (a^\dagger)^b a^c \\ &= \frac{2^{(b+c-p)/2}}{b!c!} \frac{p!}{\left(\frac{p-b-c}{2}\right)!} (a^\dagger)^b a^c \\ &= \frac{p!}{b!c! (p-b-c)!!} (a^\dagger)^b a^c \\ &\equiv F_{b,c}^p (a^\dagger)^b a^c, \end{aligned}$$

where the final expression before the bottom line is probably the simplest way of writing the coefficient. We verify using Mathematica (up to $p = 20$) that the expansion for odd p may be written

$$(a + a^\dagger)^p = \sum_{b,c|(b+c) \in 2\mathbb{Z}+1} F_{b,c}^p (a^\dagger)^b a^c.$$

Interestingly, the expression for even p may be written (again checked using Mathematica) as

$$(a + a^\dagger)^p = \sum_{b,c|(b+c) \in 2\mathbb{Z}} F_{b,c}^p (a^\dagger)^b a^c,$$

where the only difference is that the sum is now over b and c such that $(b+c)$ is even.

To do:

1. Obtain expression for matrix elements of $V(\hat{x})$.
2. Obtain expression for current per orbital.
3. Code up.