On the Harmonic Oscillator Basis for Light-Front Dynamics

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The Light-Front QCD invariant mass squared operator for a self-bound system reads,

$$\mathcal{M}^2 = \mathcal{T}_{\rm rel} + \mathcal{V}_{\rm rel} + \lambda\left(H_{\rm CM} - 2\Omega^2_{\rm CM}\right) \tag{1}$$

The relative kinetic energy is defined as:

$$\mathcal{T}_{\rm rel} = \sum_i \frac{\boldsymbol{p}_i^2}{x_i} - \left[\sum_i \boldsymbol{p}_i\right]^2 \tag{1b}$$

where $x_i \equiv \frac{p_i^+}{\sum_i p_i^+} = \frac{p_i^+}{P^+}$ is longitudinal momentum fraction. $x_i > 0, \sum_i x_i = 1$.
The potential $\mathcal{V}_{\rm rel} = \mathcal{V}_{\rm eff} + \mathcal{V}_{\rm LFQCD}$ including LF-QCD interactions and other effective potentials, is a translational invariant. Typical effective potential used in Basis Light-Front Quantized Field Theory (BLFQ) is a transverse harmonic oscillator confining potential,

$$\mathcal{V}_{\rm eff} = \kappa^4 \sum_i x_i \boldsymbol{r}_i^2 - \kappa^4 \left[\sum_i x_i \boldsymbol{r}_i\right]^2. \tag{1c}$$

Lawson term $H_{\rm CM} = \boldsymbol{P}^2 + \Omega^4_{\rm CM}\boldsymbol{R}^2$ is introduced to lift the Center-of-Mass (CM) motion in finite truncation Hilbert space, where $\boldsymbol{P}$ and $\boldsymbol{R}$ are the CM coordinate and momentum respectively:

$$\boldsymbol{P} \equiv \sum_i \boldsymbol{p}_i; \quad \boldsymbol{R} \equiv \sum_i x_i \boldsymbol{r}_i; \tag{2}$$

$[\boldsymbol{r}_i, \boldsymbol{p}_j] = \delta_{ij}\mathbf{1} \implies [\boldsymbol{R}, \boldsymbol{P}] = \mathbf{1}$.

In BLFQ, we introduce transverse harmonic oscillator (HO) plus longitudinal Plane Wave Basis, within finite truncation controlled by $N_{\max}$ and $K_{\max}$. For a single particle, the basis wavefunction is,

$$\Psi^m_n(\boldsymbol{r})e^{\mathrm{i}p^+x_+} = \mathscr{N} e^{\mathrm{i}m\theta} e^{-\frac{1}{2}\rho^2} L_n^{|m|}(\rho^2) e^{\mathrm{i}p^+x_+} \tag{3}$$

where $\rho \equiv \frac{|\boldsymbol{r}|}{\ell}, \theta = \arg \boldsymbol{r}$, HO natural length $\ell = \sqrt{\frac{\hbar}{M_{\rm HO}\Omega_{\rm HO}}}$ is a free parameter of the basis; $L_n^{|m|}(x)$ is the generalized Laguerre polynomials. The multi-particles basis is tensor space of single particle one. We adopt two truncations:

1. in transverse directions, $\sum_i(2n_i + |m_i| + 1) \leq N_{\max}$ (called $N_{\max}$ truncation);
2. We put longitudinal direction x_+ into a box with length L, hence $p^+ = \frac{2\pi n}{L}$, $n = 1, 2, 3, \cdots$ for bosons (periodic boundary condition) or $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$ for fermions (anti-periodic boundary condition). We require $\sum_i n_i = K_{\max}$ (called $K_{\max}$ truncation).

The finite Hilbert space adopting $N_{\max}$ and $K_{\max}$ truncation is denoted by $\mathcal{H}[N_{\max}, K_{\max}]$.

(Factorization Theorem [6]) *Let $\mathcal{N}$ be parton number. In $\mathcal{H}[N_{\max}, \frac{\mathcal{N}}{2}]$, each eigenstate of $\mathcal{M}^2$ factorizes as the direct product of CM state and intrinsic state,*

$$\psi = \psi_{\rm CM} \otimes \psi_{int}$$

The eigenvalue $E = E_{\text{CM}} + E_{int}$. *The CM part is a HO with natural length* $\ell/\sqrt{\mathcal{N}}$, *where* $\ell = \sqrt{\frac{\hbar}{M_{\text{HO}}\Omega_{\text{HO}}}}$ *is the natural length of the basis.*
Unfortunately, the factorization theorem does not hold for arbitrary K_{max}.

1 Momentum Fraction Weighed HO Basis (Maris Basis)

Introduce momentum fraction weighed variables (aka. "Maris variables"):

$$\boldsymbol{q}_i = \frac{\boldsymbol{p}_i}{\sqrt{x_i}}; \qquad \boldsymbol{s}_i = \sqrt{x_i}\boldsymbol{r}_i \tag{4}$$

$[\boldsymbol{s}_i, \boldsymbol{q}_j] = \delta_{ij}\mathbf{1}$ holds. The kinetic energy and confining potential in terms of Maris variables are

$$\mathcal{T}_{\text{rel}} = \sum_i \boldsymbol{q}_i^2 - \left[\sum_i \sqrt{x_i}\boldsymbol{q}_i\right]^2; \quad \mathcal{V}_{\text{eff}} = \kappa^4 \sum_i \boldsymbol{s}_i^2 - \kappa^4 \left[\sum_i \sqrt{x_i}\boldsymbol{s}_i\right]^2. \tag{5}$$

The CM variables become,

$$\boldsymbol{P} = \sum_i \sqrt{x_i}\boldsymbol{q}_i; \qquad \boldsymbol{R} = \sum_i \sqrt{x_i}\boldsymbol{s}_i \tag{6}$$

For a 2-particle system, relative momentum/coordinate may be introduced as:

$$\boldsymbol{q}_{\text{rel}} = \sqrt{x_2}\boldsymbol{q}_1 - \sqrt{x_1}\boldsymbol{q}_2, \quad \boldsymbol{s}_{\text{rel}} = \sqrt{x_2}\boldsymbol{s}_1 - \sqrt{x_1}\boldsymbol{s}_2 = \sqrt{x_1 x_2}(\boldsymbol{r}_1 - \boldsymbol{r}_2). \tag{7}$$

Kinetic energy $\mathcal{T}_{\text{rel}} = \boldsymbol{q}_{\text{rel}}^2$ Potential $\mathcal{V}_{\text{rel}} = \mathcal{V}_{\text{eff}}(\boldsymbol{s}_{\text{rel}}) + \mathcal{V}_{\text{LFQCD}}(\boldsymbol{q}_{\text{rel}})$. is only a function of relative variables. Relative variables for multi-particle system are not uniquely defined.

Introduce $\boldsymbol{q}$ representation and $\boldsymbol{s}$ representation. Let x be longitudinal momentum fraction, i.e. only consider the $\sum_i p_i^+ = P^+$ sector.

$$\hat{\boldsymbol{q}}\,|\boldsymbol{p}\rangle = \frac{\hat{\boldsymbol{p}}}{\sqrt{x}}\,|\boldsymbol{p}\rangle = \frac{\boldsymbol{p}}{\sqrt{x}}\,|\boldsymbol{p}\rangle = \boldsymbol{q}\,|\boldsymbol{p}\rangle \implies |\boldsymbol{q}\rangle = \mathcal{C}\,|\boldsymbol{p}\rangle$$

$$\begin{aligned}
&(2\pi)^3\delta^2(\boldsymbol{q} - \boldsymbol{q}')\delta(x - x') = \langle \boldsymbol{q}, x|\boldsymbol{q}', x'\rangle = |\mathcal{C}|^2 \langle \boldsymbol{p}, x|\boldsymbol{p}', x'\rangle = (2\pi)^3|\mathcal{C}|^2\delta^2(\boldsymbol{p} - \boldsymbol{p}')\delta(x - x') \\
\implies &|\mathcal{C}|^2\delta^2(\sqrt{x}\boldsymbol{q} - \sqrt{x'}\boldsymbol{q}')\delta(x - x') = \delta^2(\boldsymbol{q} - \boldsymbol{q}')\delta(x - x') \\
\implies &\mathcal{C} = \sqrt{x}e^{\mathrm{i}\phi}
\end{aligned}$$

By choosing $\phi = 0$, we fix the $\boldsymbol{q}$ representation $|\boldsymbol{q}, x\rangle = \sqrt{x}\,|\boldsymbol{p}, x\rangle$, or, $|\boldsymbol{q}\rangle = \sqrt{x}\,|\boldsymbol{p}\rangle$ for short. It can be shown $\boldsymbol{q}$-representation is complete and orthonormal,

$$\begin{aligned}
&\langle \boldsymbol{q}, x|\boldsymbol{q}', x'\rangle = (2\pi)^2\delta^2(\boldsymbol{q} - \boldsymbol{q}')(2\pi)\delta(x - x') \\
&\int \frac{\mathrm{d}^2\boldsymbol{q}}{(2\pi)^2}\int_0^1 \frac{\mathrm{d}x}{2\pi}\,|\boldsymbol{q}, x\rangle\langle \boldsymbol{q}, x| = \mathrm{Id}_3
\end{aligned} \tag{8}$$

Similarly, $\boldsymbol{s}$ representation may be defined as $|\boldsymbol{s}, x\rangle = \frac{1}{\sqrt{x}}\,|\boldsymbol{r}, x\rangle$. This is also an orthonormal complete basis.

In practice, the longitudinal coordinate is compactified to a circle $x_+ \in [-\frac{L}{2}, +\frac{L}{2}]$. Hence the momentum is discrete: $p^+ = \frac{2\pi}{L}n, (n = 1, 2, \cdots;$ or $\frac{1}{2}, \frac{3}{2}, \cdots)$. Then the orthonormality and completeness become:

$$\begin{aligned}
&\langle \boldsymbol{q}, x|\boldsymbol{q}', x'\rangle = (2\pi)^2\delta^2(\boldsymbol{q} - \boldsymbol{q}')\delta_{x,x'} \\
&\sum_x \int \frac{\mathrm{d}^2\boldsymbol{q}}{(2\pi)^2}\,|\boldsymbol{q}, x\rangle\langle \boldsymbol{q}, x| = \mathrm{Id}_3
\end{aligned} \tag{8$'$}$$

In contrast of normal coordinates, We introduce basis function with respect to Maris variables. Similarly, the single particle basis wavefunction is,

$$\Psi_n^m(\boldsymbol{s})e^{\mathrm{i}p^+x_+} = \mathscr{N}e^{\mathrm{i}m\theta}e^{-\frac{1}{2}\rho^2}L_n^{|m|}(\rho^2)e^{\frac{\mathrm{i}}{2}p^+x^-} = \Psi_n^m(\sqrt{x}\boldsymbol{r})e^{\mathrm{i}p^+x_+} \tag{9}$$

where $\rho \equiv \frac{|\boldsymbol{s}|}{\ell}, \theta = \arg \boldsymbol{s}$, $\ell = \sqrt{\frac{\hbar}{M_{\text{HO}}\Omega_{\text{HO}}}}$ is the basis natural length.

Formally, let $\alpha_\lambda(\boldsymbol{q}, x)$ be annihilation operator of Maris momentum, i.e. $\alpha^\dagger_\lambda(\boldsymbol{q}, x)\,|0\rangle \equiv |\boldsymbol{q}, x\rangle$, $a_\lambda(\boldsymbol{p}, x)$ annihilation operator of true momentum. Then $a^\dagger_\lambda(\boldsymbol{p}, x)\,|0\rangle = |\boldsymbol{p}, x\rangle = \frac{1}{\sqrt{x}}\,|\boldsymbol{q}, x\rangle = \frac{1}{\sqrt{x}}\alpha^\dagger_\lambda(\boldsymbol{q}, x)\,|0\rangle \implies a_\lambda(\boldsymbol{p}, x) = \frac{1}{\sqrt{x}}\alpha_\lambda(\boldsymbol{q}, x)$. Introduce creation/annihilation operator of Maris basis,

$$\begin{aligned} \alpha_\lambda(\boldsymbol{q}, x) &= \sum_{n,m}\Psi_n^m(\boldsymbol{q})\alpha_\lambda(n, m, x) \\ \implies a_\lambda(\boldsymbol{q}, x) &= \frac{1}{\sqrt{x}}\sum_{n,m}\Psi_n^m(\boldsymbol{q})\alpha_\lambda(n, m, x) \end{aligned} \tag{10}$$

$$\begin{aligned} \Big[\alpha_\lambda(\boldsymbol{q}, x), \alpha^\dagger_{\lambda'}(\boldsymbol{q'}, x')\Big]_\pm &= (2\pi)^2\delta^2(\boldsymbol{q}-\boldsymbol{q'})\delta_{x,x'}\delta_{\lambda,\lambda'} \\ \implies \Big[\alpha_\lambda(n, m, x), \alpha^\dagger_{\lambda'}(n, m, x')\Big]_\pm &= \delta_{n,n'}\delta_{m,m'}\delta_{x,x'}\delta_{\lambda,\lambda'} \end{aligned}$$

The HO basis wavefunction $\Psi_n^m(\boldsymbol{q})$ is normalized as:

$$\Psi_n^m(\boldsymbol{q}) \equiv \ell\sqrt{\frac{4\pi n!}{(n+|m|)!}}e^{\mathrm{i}m\phi}\rho^{|m|}e^{-\frac{\rho^2}{2}}L_n^{|m|}(\rho^2) \tag{11a}$$

where $\rho \equiv \frac{|\boldsymbol{q}|}{b}, \phi = \arg \boldsymbol{q}$, $b = \hbar\ell^{-1} = \sqrt{\hbar M_{\text{HO}}\Omega_{\text{HO}}}$ is the basis energy scale. The orthonormality and completeness hold:

$$\int \text{đ}^2\boldsymbol{q}\Psi_n^m(\boldsymbol{q})\Psi_{n'}^{m'*}(\boldsymbol{q}) = \delta_{n,n'}\delta_{m,m'} \tag{11b}$$

$$\sum_{m,n}\Psi_n^m(\boldsymbol{q})\Psi_n^{m*}(\boldsymbol{q'}) = (2\pi)^2\delta^2(\boldsymbol{q}-\boldsymbol{q'}) \tag{11c}$$

Define Maris basis,

$$|n, m, x\rangle \equiv \alpha^\dagger(n, m, x)\,|0\rangle = \int\frac{\mathrm{d}^2\boldsymbol{q}}{(2\pi)^2}\Psi_n^m(\boldsymbol{q})\,|\boldsymbol{q}, x\rangle \tag{12a}$$

The Maris basis is complete and orthonormal:

$$\begin{aligned} &\langle n', m', x'|n, m, x\rangle = \delta_{n,n'}\delta_{m,m'}\delta_{x,x'}; \\ &\sum_{n,m,x}|n, m, x\rangle\,\langle n, m, x| = \text{Id}_3. \end{aligned} \tag{12b}$$

Maris basis combined with $N_{\max}$ *truncation restores the Factorization Theorem for arbitrary* $K_{\max}$*.*

2 Brodsky and de Téramond's Impact Coordinates

In Brodsky and de Téramond's papers (See for example [4, 2, 3, 1, 5]), "internal impact coordinates" (also known as "impact variable") $\boldsymbol{b}_i$ and "relative coordinates" (momenta) $\boldsymbol{k}_i$ are defined as,

$$\boldsymbol{p}_i = x_i\boldsymbol{P} + \boldsymbol{k}_i, \quad x_i\boldsymbol{r}_i = x_i\boldsymbol{R} + \boldsymbol{b}_i \tag{13}$$

Table 1: Transition Rule of Vertex Elements from Harmonic Oscillator Basis to Maris Basis

HO basis	Maris basis
$f(\boldsymbol{p})$, $g\left(\frac{p}{x}\right)$ $(p = p_x + \mathrm{i}p_y)$	$f(\sqrt{x}\boldsymbol{q})$, $g\left(\frac{q}{\sqrt{x}}\right)$ $(q = q_x + \mathrm{i}q_y)$
$f(\boldsymbol{r})$	$f(\boldsymbol{s}/\sqrt{x})$
$a(\bar{\gamma}), b(\bar{\gamma})$	$\frac{1}{\sqrt{x}}\alpha(\bar{\gamma})$, $\frac{1}{\sqrt{x}}\beta(\bar{\gamma})$
$\int đ^2\boldsymbol{p}$	$x\int đ^2\boldsymbol{q}$
$\delta^2(\boldsymbol{p}_1 + \boldsymbol{p}_2 - \boldsymbol{p}')$	$\delta^2(\sqrt{x_1}\boldsymbol{q}_1 + \sqrt{x_2}\boldsymbol{q}_2 - \sqrt{x'}\boldsymbol{q}')$
$\Psi_n^m(\boldsymbol{p})$	$\Psi_n^m(\boldsymbol{q})$
(TM transform phase δ) $\frac{\pi}{4}$	$\arctan\sqrt{\frac{x_2}{x_1}}$

so that $\sum_i \boldsymbol{k}_i = 0, \sum_i \boldsymbol{b}_i = 0$. The authors claimed $\boldsymbol{b}_i$ and $\boldsymbol{k}_i$ is a conjugate pair. A quick check shows

$$[\boldsymbol{b}_i, \boldsymbol{k}_j] = (\delta_{ij}x_i - x_i x_j)\mathbf{1} \tag{14}$$

provided $[\boldsymbol{r}_i, \boldsymbol{p}_j] = \delta_{ij}\mathbf{1}$. Nevertheless, those authors adopted the usual identification: $\boldsymbol{k}_i^2 \to -\nabla^2_{\boldsymbol{b}_i}$ [5]. Please note that there is no way to find $\boldsymbol{k}_i$ and $\boldsymbol{b}_j$ to satisfy canonical commutation relation $[\boldsymbol{b}_i, \boldsymbol{k}_j] = \delta_{ij}\mathbf{1}$ and $\sum_i \boldsymbol{k}_i = 0, \sum_i \boldsymbol{b}_i = 0$ simultaneously. Otherwise the commutator,

$$0 = \left[\sum_i \boldsymbol{b}_i, \sum_j \boldsymbol{k}_j\right] = \sum_{i,j} \delta_{ij} = \mathcal{N}. \tag{15}$$

where $\mathcal{N}$ is the number of partons. For a system with $\mathcal{N}$ particles, there are only $\mathcal{N} - 1$ independent conjugate pairs.

Their Light-Front Holography featured the "impact variable" ζ. In 2-particle case, it's defined as,

$$\zeta = \sqrt{x(1-x)}\boldsymbol{b}. \tag{16}$$

Its multi-particle generalization is,

$$\zeta = \sqrt{\frac{x}{1-x}} \sum_{i=1}^{\mathcal{N}-1} x_i \boldsymbol{b}_i \tag{17}$$

where $x = x_{\mathcal{N}}$, assuming spectators are the first $\mathcal{N} - 1$ partons.

In 2-particle case, $x \equiv x_1, 1 - x = x_2$. In Eq. (13) & (17) of [1],

$$\mathcal{T}_{\mathrm{rel}} = \frac{\boldsymbol{k}^2}{x(1-x)} \tag{18}$$

and in Eq. 1b if $\mathcal{N} = 2$,

$$\mathcal{T}_{\mathrm{rel}} = \frac{(x_1\boldsymbol{p}_2 - x_2\boldsymbol{p}_1)^2}{x(1-x)} = \frac{\boldsymbol{p}_{\mathrm{rel}}^2}{x(1-x)} = \boldsymbol{q}_{\mathrm{rel}}^2 \tag{19}$$

So the relative momentum $\boldsymbol{k} = \boldsymbol{p}_{\mathrm{rel}} \equiv x_2\boldsymbol{p}_1 - x_1\boldsymbol{p}_2 = \sqrt{x(1-x)}\boldsymbol{q}_{\mathrm{rel}}$. The relative coordinate $\boldsymbol{b}$ is known problematic in above discussion. Following Brodsky and de Téramond's definition, $b = x(1-x)(\boldsymbol{r}_1 - \boldsymbol{r}_2) = x(1-x)\boldsymbol{r}_{\mathrm{rel}}$, then $\zeta = x(1-x)\boldsymbol{s}_{\mathrm{rel}}$. But if we accept the conventional definition of relative coordinate,

$\boldsymbol{b} = \boldsymbol{r}_1 - \boldsymbol{r}_2 = \boldsymbol{r}_{\text{rel}}$, such that $[\boldsymbol{b}, \boldsymbol{k}] = \boldsymbol{1}$, then Maris relative coordinate is exactly impact variable $\boldsymbol{s}_{\text{rel}} = \zeta$. $\boldsymbol{q}_{\text{rel}} \to \mathrm{i}\nabla_{\boldsymbol{s}_{\text{rel}}} = \mathrm{i}\nabla_\zeta$; $\mathcal{T}_{\text{rel}} = -\nabla_\zeta^2$.

The ground state of AdS/QCD soft-wall model is a HO wavefunction $\phi_n^m(z)$. In LF Holography, the fifth dimension z is mapped to the impact variable ζ [1]. By the above identification $\boldsymbol{s}_{\text{rel}} = \zeta$, the Maris basis wavefunction is identical with the soft-wall model solution (except that one is a single particle basis, another is pure intrinsic wavefunction).

The multi-particle comparison is not available, because the relative Maris variables are not uniquely defined. It's possible to introduce relative coordinates folloing Eq. (13), for example:

$$\boldsymbol{q}_i^{\text{rel}} = \frac{\boldsymbol{q}_i}{\sqrt{1-x_i}} - \sqrt{\frac{x_i}{1-x_i}}\boldsymbol{P}, \qquad \boldsymbol{s}_i^{\text{rel}} = \frac{\boldsymbol{s}_i}{\sqrt{1-x_i}} - \sqrt{\frac{x_i}{1-x_i}}\boldsymbol{R}$$

3 Talmi-Moshinsky Transform of Maris Basis

Now consider a basis generated by Hamiltonian

$$H = \boldsymbol{q}^2 + \boldsymbol{s}^2;$$

The eigenstates are $\{\,|n,m\rangle\}$. In "momentum" $\boldsymbol{q}$ representation, the wavefunction is

$$\Psi_n^m(\boldsymbol{q}) = q^{|m|} e^{-q^2/2} e^{\mathrm{i}m\phi} L_n^{|m|}(q^2)$$

$q = |\boldsymbol{q}|, \phi = \arg \boldsymbol{q}$.

Generating function of $\Psi_n^m(\boldsymbol{p})$ is,

$$e^{-\frac{1}{2}\boldsymbol{p}^2 + 2\boldsymbol{p}\cdot\boldsymbol{z} - \boldsymbol{z}^2} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{(-1)^n}{\sqrt{4\pi(n+|m|)!n!}} \Psi_n^m(\boldsymbol{p}) e^{-\mathrm{i}m\theta} z^{2n+|m|} \tag{20}$$

where, $z = |\boldsymbol{z}|, \theta = \arg \boldsymbol{z}$.

If we define,

$$\begin{aligned} \boldsymbol{Q} &= \frac{\sqrt{x_1}\boldsymbol{q_1} + \sqrt{x_2}\boldsymbol{q_2}}{\sqrt{x_1+x_2}} = \frac{\boldsymbol{P}}{\sqrt{x_1+x_2}}, \quad \boldsymbol{q} = \frac{\sqrt{x_2}\boldsymbol{q_1} - \sqrt{x_1}\boldsymbol{q_2}}{\sqrt{x_1+x_2}} = \frac{\boldsymbol{P}_{\text{rel}}}{\sqrt{\frac{x_1x_2}{x_1+x_2}}} \\ \boldsymbol{\zeta} &= \frac{\sqrt{x_1}\boldsymbol{z_1} + \sqrt{x_2}\boldsymbol{z_2}}{\sqrt{x_1+x_2}}, \qquad \boldsymbol{z} = \frac{\sqrt{x_2}\boldsymbol{z_1} - \sqrt{x_1}\boldsymbol{z_2}}{\sqrt{x_1+x_2}} \end{aligned} \tag{21}$$

identity

$$(-\tfrac{1}{2}\boldsymbol{q}_1^2 + 2\boldsymbol{q}_1\cdot\boldsymbol{z}_1 - \boldsymbol{z}_1^2) + (-\tfrac{1}{2}\boldsymbol{q}_1^2 + 2\boldsymbol{q}_2\cdot\boldsymbol{z}_2 - \boldsymbol{z}_2^2) = (-\tfrac{1}{2}\boldsymbol{Q}^2 + 2\boldsymbol{Q}\cdot\boldsymbol{\zeta} - \boldsymbol{\zeta}^2) + (-\tfrac{1}{2}\boldsymbol{q}^2 + 2\boldsymbol{q}\cdot\boldsymbol{z} - \boldsymbol{z}^2)$$

holds.

Therefore,

$$\begin{aligned} &\sum_{n_1,m_1,n_2,m_2} \frac{(-1)^{n_1+n_2}}{4\pi\sqrt{(n_1+|m_1|)!n_1!(n_2+|m_2|)!n_2!}} \Psi_{n_1}^{m_1}(\boldsymbol{q_1})\Psi_{n_2}^{m_2}(\boldsymbol{q_2}) e^{-\mathrm{i}m_1\theta_1 - \mathrm{i}m_2\theta_2} z_1^{2n_1+|m_1|} z_2^{2n_2+|m_2|} \\ =& \sum_{N,M,n,m} \frac{(-1)^{N+n}}{4\pi\sqrt{(N+|M|)!N!(n+|m|)!n!}} \Psi_N^M(\boldsymbol{Q})\Psi_n^m(\boldsymbol{q}) e^{-\mathrm{i}M\Theta - \mathrm{i}m\theta} \zeta^{2N+|M|} z^{2n+|m|} \end{aligned}$$

And ζ, z, Θ, θ are functions of $z_1, z_2, \theta_1, \theta_2$, eps. $\zeta, z, e^{\mathrm{i}\Theta}, e^{\mathrm{i}\theta}$ are polynomials of $z_1, z_2, e^{\mathrm{i}\theta_1}, e^{\mathrm{i}\theta_2}$. Therefore, we can expand right-hand side in terms of $z_1, z_2, e^{\mathrm{i}\theta_1}, e^{\mathrm{i}\theta_2}$, and identify each term on the left-hand side, i.e.

$$\begin{aligned} &\frac{(-1)^{n_1+n_2}}{4\pi\sqrt{(n_1+|m_1|)!n_1!(n_2+|m_2|)!n_2!}} \Psi_{n_1}^{m_1}(\boldsymbol{q_1})\Psi_{n_2}^{m_2}(\boldsymbol{q_2}) e^{-\mathrm{i}m_1\theta_1 - \mathrm{i}m_2\theta_2} z_1^{2n_1+|m_1|} z_2^{2n_2+|m_2|} \\ =& {\sum_{N,M,n,m}}' \frac{(-1)^{N+n}}{4\pi\sqrt{(N+|M|)!N!(n+|m|)!n!}} \Psi_N^M(\boldsymbol{Q})\Psi_n^m(\boldsymbol{q}) e^{-\mathrm{i}M\Theta - \mathrm{i}m\theta} \zeta^{2N+|M|} z^{2n+|m|} \end{aligned}$$

$\sum'$ sums over selected (N, M, n, m) that makes $e^{-\mathrm{i}M\Theta - \mathrm{i}m\theta}\zeta^{2N+|M|}z^{2n+|m|} \propto e^{-\mathrm{i}m_1\theta_1 - \mathrm{i}m_2\theta_2} z_1^{2n_1+|m_1|} z_2^{2n_2+|m_2|}$. Since $\zeta, z, e^{\mathrm{i}\Theta}, e^{\mathrm{i}\theta}$ are only polynomials of $z_1, z_2, e^{\mathrm{i}\theta_1}, e^{\mathrm{i}\theta_2}$, power counting works here. The degree of polynomials on the left-hand side and a typical term of right-hand side is $2n_1 + |m_1| + 2n_2 + |m_2|$ and $2N + |M| + 2n + |m|$ respectively. Hence, $0 \le 2N + |M| + 2n + |m| \le 2n_1 + |m_1| + 2n_2 + |m_2|$. It implies the right-hand series is finite.

Define Talmi-Moshinsky coefficients (aka TM Bracket),

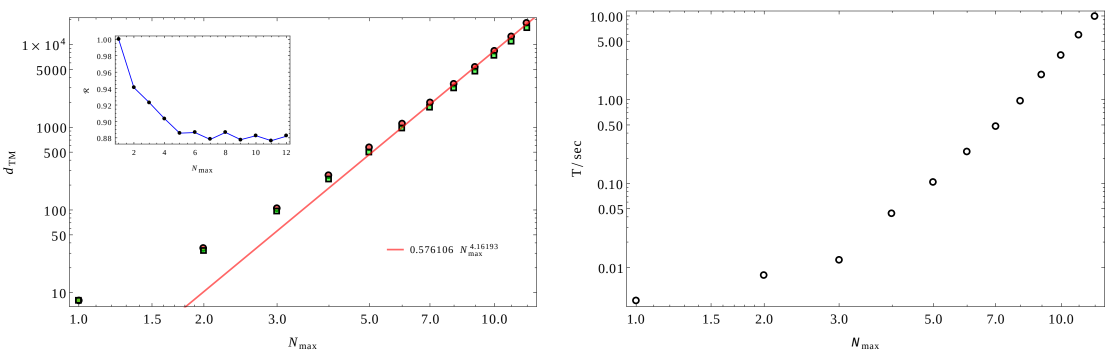
$$\Psi_{n_1}^{m_1}(\boldsymbol{q}_1)\Psi_{n_2}^{m_2}(\boldsymbol{q}_2) = \sum_{NMnm} \mathcal{M}_{n_1m_1n_2m_2}^{NMnm}(x_1, x_2)\Psi_N^M(\boldsymbol{Q})\Psi_n^m(\boldsymbol{q}) \tag{22}$$

where $\boldsymbol{Q} = \frac{\sqrt{x_1}\boldsymbol{q}_1 + \sqrt{x_2}\boldsymbol{q}_2}{\sqrt{x_1+x_2}}, \boldsymbol{q} = \frac{\sqrt{x_2}\boldsymbol{q}_1 - \sqrt{x_1}\boldsymbol{q}_2}{\sqrt{x_1+x_2}}$. Bracket form $\mathcal{M}_{n_1m_1n_2m_2}^{NMnm} \equiv \langle NMnm|n_1m_1n_2m_2\rangle$ sometimes is favored though not Dirac bracket. They're exactly the same coefficients used in 2D HO wavefunctions.

$$\begin{aligned}
&\mathcal{M}_{n_1m_1n_2m_2}^{N_1M_1N_2M_2} = \delta_{2n_1+|m_1|+2n_2+|m_2|}^{2N_1+|M_1|+2N_2+|M_2|}\delta_{m_1+m_2}^{M_1+M_2}(-1)^{N_1+N_2-n_1-n_2}\sqrt{\frac{(n_1+|m_1|)!(n_2+|m_2|)!n_1!n_2!}{(N_1+|M_1|)!(N_2+|M_2|)!N_1!N_2!}} \\
&\cdot (\sin\delta)^{2n_2+|m_2|}(\cos\delta)^{2n_1+|m_1|}(-1)^{N_2+\frac{1}{2}(|M_2|+M_2)}(\tan\delta)^{M_2}\cdot \\
&\sum_{\gamma_1=0}^{v_1}\sum_{\gamma_2=0}^{v_2}\sum_{\beta_1=0}^{\gamma_1}\sum_{\beta_2=0}^{\gamma_2}\sum_{\beta_3=0}^{V_2}\sum_{\beta=0}^{M_2}\cdot\Bigg[(-1)^{\beta_1-\beta_2+\beta}(\tan\delta)^{\beta_1-\beta_2+\beta}\binom{M_1}{v_1-v_2+m_1+\gamma_2-\gamma_1-\beta}\binom{M_2}{\beta} \\
&\binom{V_2}{\beta_1,\beta_2,\beta_3,V_2-\beta_1-\beta_2-\beta_3}\binom{v_1+v_2-V_2}{\gamma_1-\beta_1,\gamma_2-\beta_2,v_1-\gamma_1-\beta_3,v_2-\gamma_2-V_2+\beta_1+\beta_2+\beta_3}\Bigg]
\end{aligned} \tag{23}$$

where $v_i = n_i + \frac{1}{2}(m_i - |m_i|), V_i = N_i + \frac{1}{2}(M_i - |M_i|), i = 1, 2;\ \delta = \arctan\sqrt{\frac{x_2}{x_1}}$. The multinomial coefficients $\binom{n,}{m_1,m_2,\cdots,m_k}$ satisfies $m_1 + m_2 + \cdots m_k = n,\ 0 \le m_i \le n, i = 1, 2, \cdots k$. The binomial coefficients however are the generalized ones, $\binom{n}{m} = \frac{n(n-1)\cdots(n-m+1)}{m!}, m \ge 0$ and $\binom{n}{0} = 1$.

Two delta functions $\delta_{m_1+m_2}^{M_1+M_2}, \delta_{2n_1+|m_1|+2n_2+|m_2|}^{2N_1+|M_1|+2N_2+|M_2|}$ suffice to estimate if a TM coefficient is zero. There are of course accidental zeros. The estimation efficiency is $> 95\%$.



(a) The number of estimated nonzeros (Red) and actual nonzeros (green). $\mathcal{R}$ is their ratio.

(b) The timing of calculation of TM Coefficients.

4 Basis Wavefunction Integrals

The Basis LFQCD vertices do not directly depend on $\boldsymbol{p}$. Therefore, the vertices (except kinetic terms, CM term, lawson term and the effective potential) keep unchanged when Maris basis is used. However, the basis wavefunction integrals are different. In this section, we present calculation of wavefunction integrals. All the calculation is done by assumming *conservation of longitudinal momentum:* $\sum_i x_i = \sum_j x_j'$.

Let n, m, k be positive integers, $q = q_x + \mathrm{i}q_y$ be the complex representation of 2D vector $\boldsymbol{q} = q_x\boldsymbol{e}_x + q_y\boldsymbol{e}_y$ and $\text{đ}^2p \equiv \frac{\mathrm{d}^2p}{(2\pi)^2}$.

Elementary integrals:

$$\mathbb{I}^{(k)}_{nm} \equiv \ell^{k+1}\int \text{đ}^2q\, q^k\Psi^m_n(q) = (-1)^n\frac{2^k}{k!}\sqrt{\frac{(n+k)!}{\pi n!}}\delta_{m+k,0} \tag{24a}$$

$$\mathbb{I}^{(0)}_{nmn'm'} \equiv \int \text{đ}^2q\ \Psi^{m'*}_{n'}(q)\Psi^m_n(q) = \delta_{n,n'}\delta_{m,m'} \tag{24b}$$

$$\mathbb{I}^{(1)}_{nmn'm'} \equiv \ell\int \text{đ}^2q\, q\Psi^{m'*}_{n'}(q)\Psi^m_n(q) = \delta_{m',m+1}\cdot\begin{cases}\sqrt{n+|m+1|}\delta_{n,n'} - \sqrt{n}\delta_{n',n-1} & m\ge 0\\ \sqrt{n+|m|}\delta_{n,n'} - \sqrt{n+1}\delta_{n',n+1} & m<0.\end{cases} \tag{24c}$$

where $\ell = \sqrt{\frac{\hbar}{M_{\text{HO}}\Omega_{\text{HO}}}}$ is the natural length of the basis wavefunctions Ψ^m_n.

Wavefunction Integrals of $q_1 + q_2 \to q'$:

$$\int \text{đ}^2q_1\,\text{đ}^2q_2\,\text{đ}^2q'\ (2\pi)^2\delta^2(\sqrt{x_1}q_1 + \sqrt{x_2}q_2 - \sqrt{x'}q')\cdot q_1\cdot\Psi^{m_1}_{n_1}(q_1)\Psi^{m_2}_{n_2}(q_2)\Psi^{m'*}_{n'}(q')$$
$$=\frac{\delta_{m_1+m_2,m'-1}}{\ell^2(x_1+x_2)^{\frac{3}{2}}}\left[\sqrt{x_1}\sum_{N=\max(n'-1,0)}^{\min(\nu,n'+1)}\mathcal{M}^{N,m'-1,\nu-N,0}_{n_1,m_1,n_2,m_2}\mathbb{I}^{(0)}_{\nu-N,0}\mathbb{I}^{(1)}_{N,m'-1,n',m'} + \vartheta(n)\sqrt{x_2}\mathcal{M}^{n',m',n,-1}_{n_1,m_1,n_2,m_2}\mathbb{I}^{(1)}_{n,-1}\right] \tag{25a}$$
$$\nu = n_1+n_2+\tfrac{1}{2}(|m_1|+|m_2|-|m_1+m_2|),\ n = n_1+n_2-n'+\tfrac{1}{2}(|m_1|+|m_2|-1-|m'|)\ge 0$$

$$\int \text{đ}^2q_1\,\text{đ}^2q_2\,\text{đ}^2q'\ (2\pi)^2\delta^2(\sqrt{x_1}q_1 + \sqrt{x_2}q_2 - \sqrt{x'}q')\cdot q_2\cdot\Psi^{m_1}_{n_1}(q_1)\Psi^{m_2}_{n_2}(q_2)\Psi^{m'*}_{n'}(q')$$
$$=\frac{\delta_{m_1+m_2,m'-1}}{\ell^2(x_1+x_2)^{\frac{3}{2}}}\left[\sqrt{x_2}\sum_{N=\max(n'-1,0)}^{\min(\nu,n'+1)}\mathcal{M}^{N,m'-1,\nu-N,0}_{n_1,m_1,n_2,m_2}\mathbb{I}^{(0)}_{\nu-N,0}\mathbb{I}^{(1)}_{N,m'-1,n',m'} - \vartheta(n)\sqrt{x_1}\mathcal{M}^{n',m',n,-1}_{n_1,m_1,n_2,m_2}\mathbb{I}^{(1)}_{n,-1}\right] \tag{25b}$$
$$\nu = n_1+n_2+\tfrac{1}{2}(|m_1|+|m_2|-|m_1+m_2|),\ n = n_1+n_2-n'+\tfrac{1}{2}(|m_1|+|m_2|-1-|m'|)\ge 0$$

$$\int \text{đ}^2q_1\,\text{đ}^2q_2\,\text{đ}^2q'\ (2\pi)^2\delta^2(\sqrt{x_1}q_1 + \sqrt{x_2}q_2 - \sqrt{x'}q')\cdot q'\cdot\Psi^{m_1}_{n_1}(q_1)\Psi^{m_2}_{n_2}(q_2)\Psi^{m'*}_{n'}(q')$$
$$=\frac{\delta_{m_1+m_2,m'-1}}{\ell^2(x_1+x_2)}\sum_{N=\max(n'-1,0)}^{\min(\nu,n'+1)}\mathcal{M}^{N,m'-1,\nu-N,0}_{n_1,m_1,n_2,m_2}\mathbb{I}^{(0)}_{\nu-N,0}\ \mathbb{I}^{(1)}_{N,m'-1,n',m'} \tag{25c}$$
$$\nu = n_1+n_2+\tfrac{1}{2}(|m_1|+|m_2|-|m_1+m_2|)$$

$$\int \text{đ}^2q_1\,\text{đ}^2q_2\,\text{đ}^2q'\ (2\pi)^2\delta^2(\sqrt{x_1}q_1 + \sqrt{x_2}q_2 - \sqrt{x'}q')\cdot\Psi^{m_1}_{n_1}(q_1)\Psi^{m_2}_{n_2}(q_2)\Psi^{m'*}_{n'}(q')$$
$$=\vartheta(n)\frac{\delta_{m_1+m_2,m'}}{\ell(x_1+x_2)}\mathcal{M}^{n',m',n,0}_{n_1,m_1,n_2,m_2}\mathbb{I}^{(0)}_{n,0} \tag{25d}$$
$$n = n_1+n_2-n'+\tfrac{1}{2}(|m_1|+|m_2|-|m_1+m_2|)\ge 0$$

Wavefunction Integrals of $q_1 + q_2 + q_3 \to q'$ and $q_1 + q_2 \to q'_1 + q'_2$:

$$\int \text{đ}^2q_1\,\text{đ}^2q_2\,\text{đ}^2q_3\,\text{đ}^2q'\ (2\pi)^2\delta^2(\sqrt{x_1}q_1 + \sqrt{x_2}q_2 + \sqrt{x_3}q_3 - \sqrt{x'}q')\Psi^{m_1}_{n_1}(q_1)\Psi^{m_2}_{n_2}(q_2)\Psi^{m_3}_{n_3}(q_3)\Psi^{m'*}_{n'}(q')$$
$$=\frac{\delta_{m_1+m_2+m_3,m'}}{\ell^2(x_1+x_2+x_3)}\sum_{N=\max(0,-\chi)}^{\xi}\mathcal{M}^{N,m_1+m_2,\xi-N,0}_{n_1,m_1,n_2,m_2}(x_1,x_2)\mathcal{M}^{n',m',\chi+N,0}_{N,m_1+m_2,n_3,m_3}(x_1+x_2,x_3)\ \mathbb{I}^{(0)}_{\xi-N,0}\ \mathbb{I}^{(0)}_{\chi+N,0} \tag{26a}$$
$$\xi = n_1+n_2+\tfrac{1}{2}(|m_1|+|m_2|-|m_1+m_2|),\ \chi = n_3-n'+\tfrac{1}{2}(|m_1+m_2|+|m_3|-|m'|)$$

$$
\begin{aligned}
&\int đ^2 q_1\, đ^2 q_2\, đ^2 q_1'\, đ^2 q_2'\ (2\pi)^2 \delta^2(\sqrt{x_1} q_1 + \sqrt{x_2} q_2 - \sqrt{x_1'} q_1' - \sqrt{x_2'} q_2') \Psi_{n_1}^{m_1}(q_1) \Psi_{n_2}^{m_2}(q_2) \Psi_{n_1'}^{m_1'*}(q_3') \Psi_{n_2'}^{m_2'*}(q_2') \\
&= \frac{\delta_{m_1+m_2, m_1'+m_2'}}{\ell^2(x_1+x_2)} \sum_{N=0}^{\min(\xi,\chi)} \mathcal{M}_{n_1,m_1,n_2,m_2}^{N,m_1+m_2,n,0} \mathcal{M}_{n_1',m_1',n_2',m_2'}^{N,m_1+m_2,n',0}\ \mathbb{I}_{n,0}^{(0)}\ \mathbb{I}_{n',0}^{(0)} \\
&\xi = n_1 + n_2 + \tfrac{1}{2}(|m_1| + |m_2| - |m_1+m_2|), \chi = n_1' + n_2' + \tfrac{1}{2}(|m_1'| + |m_2'| - |m_1'+m_2'|); \\
&n = \xi - N, n' = \chi - N
\end{aligned} \tag{26b}
$$

expectation value of operator $\boldsymbol{q}^2, \boldsymbol{s}^2, \boldsymbol{q_1} \cdot \boldsymbol{q_2}, \boldsymbol{s_1} \cdot \boldsymbol{s_2}$:

$$
\begin{aligned}
&\left\langle n', m' \left| \boldsymbol{q}^2/(2\pi)^2 \right| n, m \right\rangle = \int đ^2 q\ \boldsymbol{q}^2\ \Psi_{n'}^{m'*}(q) \Psi_n^m(q) \\
=&\ell^{-2} \delta_{m,m'} \left(\delta_{n,n'}(2n + |m| + 1) - \delta_{n',n+1} \sqrt{n'(n' + |m'|)} - \delta_{n,n'+1} \sqrt{n(n+|m|)} \right)
\end{aligned} \tag{27a}
$$

$$
\begin{aligned}
&\left\langle n', m' \left| \boldsymbol{s}^2/(2\pi)^2 \right| n, m \right\rangle = \int đ^2 q\ \boldsymbol{s}^2\ \Psi_{n'}^{m'*}(q) \Psi_n^m(q) \\
=&\ell^{2} \delta_{m,m'} \left(\delta_{n,n'}(2n + |m| + 1) + \delta_{n',n+1} \sqrt{n'(n' + |m'|)} + \delta_{n,n'+1} \sqrt{n(n+|m|)} \right)
\end{aligned} \tag{27b}
$$

$$
\begin{aligned}
&\left\langle n_1' m_1' n_2' m_2' | 2\boldsymbol{q_1} \cdot \boldsymbol{q_2}/(2\pi)^4 | n_1 m_1 n_2 m_2 \right\rangle = \int đ^2 q_1\, đ^2 q_2 \cdot 2\boldsymbol{q_1} \cdot \boldsymbol{q_2} \Psi_{n_1}^{m_1}(q_1) \Psi_{n_2}^{m_2}(q_2) \Psi_{n_1'}^{m_1'*}(q_1) \Psi_{n_2'}^{m_2'*}(q_2) \\
&= \ell^{-2} \left(f_{n_1,m_1,n_1',m_1'} f_{n_2',m_2',n_2,m_2} \delta_{m_1+1,m_1'} \delta_{m_2'+1,m_2} + f_{n_1',m_1',n_1,m_1} f_{n_2,m_2,n_2',m_2'} \delta_{m_1'+1,m_1} \delta_{m_2+1,m_2'} \right)
\end{aligned} \tag{27c}
$$

$$
\begin{aligned}
&\left\langle n_1' m_1' n_2' m_2' | 2\boldsymbol{s_1} \cdot \boldsymbol{s_2}/(2\pi)^4 | n_1 m_1 n_2 m_2 \right\rangle = \int đ^2 q_1\, đ^2 q_2 \cdot 2\boldsymbol{s_1} \cdot \boldsymbol{s_2} \Psi_{n_1}^{m_1}(q_1) \Psi_{n_2}^{m_2}(q_2) \Psi_{n_1'}^{m_1'*}(q_1) \Psi_{n_2'}^{m_2'*}(q_2) \\
&= \ell^2 (-1)^{n_1+n_2-n_1'-n_2'+\frac{1}{2}(|m_1|+|m_2|-|m_1'|-|m_2'|)} \\
&\left(f_{n_1,m_1,n_1',m_1'} f_{n_2',m_2',n_2,m_2} \delta_{m_1+1,m_1'} \delta_{m_2'+1,m_2} + f_{n_1',m_1',n_1,m_1} f_{n_2,m_2,n_2',m_2'} \delta_{m_1'+1,m_1} \delta_{m_2+1,m_2'} \right)
\end{aligned} \tag{27d}
$$

where,

$$
f_{n,m,n',m'} = \begin{cases} \delta_{n,n'} \sqrt{n + |m+1|} - \delta_{n',n-1} \sqrt{n} & (m \geq 0) \\ \delta_{n,n'} \sqrt{n + |m|} - \delta_{n',n+1} \sqrt{n+1} & (m < 0) \end{cases}
$$

5 Boost Invariance and Intrinsic Operators

In Light-Front dynamics, transverse boosts are kinematical:

$$
\boldsymbol{p} \to \boldsymbol{p} + p^+ \boldsymbol{\beta} \equiv \boldsymbol{p} + x\boldsymbol{C}, \quad \boldsymbol{q} \to \boldsymbol{q} + \sqrt{x} \boldsymbol{C} \tag{28}
$$

where $x = p^+/P^+$ is momentum fraction, P^+ is the total longitudinal momentum of the system. Because of longitudinal momentum conservation, P^+ is a constant for each longitudinal sector.

Consider two particles with momenta $\{x_1, \boldsymbol{q_1}\}$ and $\{x_2, \boldsymbol{q_2}\}$ respectively. The system can also be expressed in terms of intrinsic momentum (relative momentum) and CM momentum (See Eq. (21)),

$$
\boldsymbol{Q} = \frac{\sqrt{x_1} \boldsymbol{q_1} + \sqrt{x_2} \boldsymbol{q_2}}{\sqrt{x_1 + x_2}}, \quad \boldsymbol{q} = \frac{\sqrt{x_2} \boldsymbol{q_1} - \sqrt{x_1} \boldsymbol{q_2}}{\sqrt{x_1 + x_2}} \tag{29}
$$

It can be shown that under transverse boost,

$$
\boldsymbol{Q} \to \boldsymbol{Q} + \sqrt{x_1 + x_2} \boldsymbol{C}, \quad \boldsymbol{q} \to \boldsymbol{q} \tag{30}
$$

i.e. the intrinsic part is boost invariant whereas the CM part is not. Physical operators should be boost invariants. This means, physical operators can be constructed from boost invariant variables, such as intrinsic momentum (relative momentum). In reality, we also consider boost non-invariant operators such as $\mathcal{H}_{\text{CM}}$. But we limited ourselves to the operators that can be written as the superposition of a boost invariant and a CM part. The canonical example is kinetic energy operator $\mathcal{T} = \mathcal{T}_{intr} + \mathcal{T}_{\text{CM}}$.

For many-particle system, intrinsic momenta defined by (See also Eq. (13)),

$$\begin{aligned} &\boldsymbol{k}_i = \boldsymbol{p}_i - \frac{x_i}{x}\boldsymbol{P} \equiv \boldsymbol{p}_i - y_i\boldsymbol{P}, \qquad (\boldsymbol{P} = \sum_i \boldsymbol{p_i}, \quad x = \sum_i x_i) \\ &\boldsymbol{\kappa}_i = \boldsymbol{q}_i - \sqrt{\frac{x_i}{x}}\boldsymbol{Q} \equiv \boldsymbol{q}_i - \sqrt{y_i}\boldsymbol{Q}, \quad (\kappa_i = \boldsymbol{k}_i/\sqrt{x_i}) \end{aligned} \tag{31}$$

are also boost invariants.

It can be shown, for Maris Basis Talmi-Moshinsky Transform separates the CM wavefunction and the boost invariant intrinsic wavefunction in the basis. Note that this is not true for naive two dimensional HO basis, although TM transform also separates the CM wavefunction. In the naive two dimensional HO basis, the relative momentum,

$$\begin{aligned} &\boldsymbol{p}_{\text{REL}} \equiv \frac{M_2\boldsymbol{p_1} - M_1\boldsymbol{p_2}}{M_1 + M_2} = \frac{b_2^2\boldsymbol{p_1} - b_1^2\boldsymbol{p_2}}{b_1^2 + b_2^2} = \tfrac{1}{2}(\boldsymbol{p_1} - \boldsymbol{p_2}) \\ &\boldsymbol{p}_{\text{REL}} \to \boldsymbol{p}_{\text{REL}} + \tfrac{1}{2}(x_1 - x_2)\boldsymbol{C} \end{aligned}$$

is not a boost invariant, where $b = \sqrt{M\Omega}$ is the HO basis energy scale (basis parameter), which is usually fixed for all particles.

The fact that physical operators are boost invariants can simplifies the calculation. The following examples can be found useful in BLFQ calculations.

matrix elements of $V_{qg\to q}$ The matrix elements of $V_{qg\to q}$ have the structure as $\left(\frac{p_1}{p^+} - \frac{k}{k^+}\right)$, where p_1, k are complex transverse momenta. This structure is clearly boost invariant. It implies, $V_{qg\to q}(p_1, k; p_2) = V_{qg\to q}(q)$ where q is the intrinsic momentum of the $q + g$ sector (the two-body sector). The matrix elements of $V_{qg\to q}$ are,

$$\begin{aligned} &\langle n_2, m_2|V_{qg\to q}|n_1, m_1, n_k, m_k\rangle \\ =&\sum_{NMnm} \mathcal{M}^{N,M,n,m}_{n_1,m_1,n_k,m_k} \int đ^2Q\, đ^2q\, đ^2q_2 (2\pi)^2\delta^2(\sqrt{X}Q - \sqrt{x_2}q_2)\bar{V}_{qg\to q}(q)\Psi^M_N(Q)\Psi^m_n(q)\Psi^{m_2*}_{n_2}(q_2) \\ =&\frac{1}{x_2}\sum_{NMnm} \mathcal{M}^{N,M,n,m}_{n_1,m_1,n_k,m_k}\delta_{N,n_2}\delta_{M,m_2}\int đ^2q\ \bar{V}_{qg\to q}(q)\Psi^m_n(q) \end{aligned} \tag{32}$$

where $\bar{V}_{qg\to q} \equiv V_{qg\to q}/(2\pi)^2\delta^2(p_1+k-p_2)$. Longitudinal momentum conservation implies $x_2 = x_1+x_k \equiv X$. In single particle wavefunction integral (25a), there are two parts, corresponding to CM part (the first part) and intrinsic part (the second part). In matrix elements, the CM part will be canceled eventually, left only the intrinsic part, as we have shown above [1].

the kinetic energy The (intrinsic) kinetic energy is also a boost invariant operator. Consider the two-body case, $\mathcal{T}_{intr} = \frac{\boldsymbol{p_1}^2}{x_1} + \frac{\boldsymbol{p_2}^2}{x_2} - \frac{(\boldsymbol{p_1}+\boldsymbol{p_2})^2}{x_1+x_2} = \left(\frac{\sqrt{x_2}\boldsymbol{q_1} - \sqrt{x_1}\boldsymbol{q_2}}{\sqrt{x_1+x_2}}\right)^2 \equiv \boldsymbol{q}^2$. We have shown in last section that the kinetic energy operator can be computed from single particle integrals (See Eq.(27)). It can also be computed using TM transform,

$$\begin{aligned} &\langle n_1', m_1', n_2', m_2'|\mathcal{T}_{intr}|n_1, m_1, n_2, m_2\rangle \\ =&\sum_{NMnm}\ \sum_{N'M'n'm'} \mathcal{M}^{NMnm}_{n_1m_1n_2m_2}\mathcal{M}^{N'M'n'm'}_{n_1'm_1'n_2'm_2'}\delta_{N,N'}\delta_{M,M'}\int đ^2q\ \boldsymbol{q}^2\Psi^m_n(q)\Psi^{m'*}_{n'}(q) \end{aligned} \tag{33}$$

[1] This phenomenon is noticed by Dr. Maris.

This expression is more compact, and can be used to estimate if the matrix element is zero. Of course, computing TM coefficient in run-time is much slower. Similarly,

$$\begin{aligned}
&\langle n'_1, m'_1, n'_2, m'_2|\mathcal{T}_{\text{CM}}|n_1, m_1, n_2, m_2\rangle \\
&= \sum_{NMnm} \sum_{N'M'n'm'} \mathcal{M}^{NMnm}_{n_1m_1n_2m_2} \mathcal{M}^{N'M'n'm'}_{n'_1m'_1n'_2m'_2} \delta_{n,n'}\delta_{m,m'} \int \text{đ}^2Q\, \boldsymbol{Q}^2 \Psi^M_N(Q)\Psi^{M'*}_{N'}(Q)
\end{aligned} \tag{34}$$

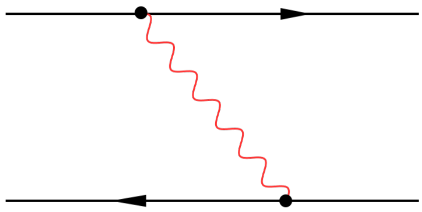


Figure 1

the energy denominator The Feynman diagram of the operator is shown in Fig. 1.

$$I = \int \text{đ}^2q_1\,\text{đ}^2q_2\,\text{đ}^2q'_1\,\text{đ}^2q'_2\, \frac{(2\pi)^2\delta^2(\sqrt{x_1}q_1+\sqrt{x_2}q_2-\sqrt{x'_1}q'_1-\sqrt{x'_2}q'_2)}{\frac{x_1\boldsymbol{q}_1^2+m_f^2}{x_1} - \frac{x'_1\boldsymbol{q}'^2_1+m_f^2}{x'_1} - \frac{(\sqrt{x_1}\boldsymbol{q}_1-\sqrt{x'_1}\boldsymbol{q}'_1)^2}{x_1-x'_1}} \Psi^{m_1}_{n_1}(q_1)\Psi^{m_2}_{n_2}(q_2)\Psi^{m'_1*}_{n'_1}(q'_1)\Psi^{m'_2*}_{n'_2}(q'_2) \tag{35}$$

with the longitudinal momentum conservation $X \equiv x_1 + x_2 = x'_1 + x'_2 \equiv X'$. Introduce a boost invariant $\boldsymbol{k} \equiv \sqrt{x'_1}\boldsymbol{q}_1 - \sqrt{x_1}\boldsymbol{q}'_1$. It can be shown the energy denominator can be written as,

$$D \equiv \frac{x_1\boldsymbol{q}_1^2 + m_f^2}{x_1} - \frac{x'_1\boldsymbol{q}'^2_1 + m_f^2}{x'_1} - \frac{(\sqrt{x_1}\boldsymbol{q}_1 - \sqrt{x'_1}\boldsymbol{q}'_1)^2 + \mu^2}{x_1 - x'_1} = -\frac{\boldsymbol{k}^2}{x_1 - x'_1} + \frac{m_f^2}{x_1} - \frac{m_f^2}{x'_1} - \frac{\mu^2}{x_1 - x'_1}.$$

Hence the energy denominator is also a boost invariant. On the other hand, within CM and intrinsic parameters, the only boost invariant momenta are $\boldsymbol{q}, \boldsymbol{q}', \boldsymbol{Q} - \boldsymbol{Q}'$. By TM transform,

$$\begin{aligned}
I = &\sum_{NMnm} \sum_{N'M'n'm'} \mathcal{M}^{NMnm}_{n_1m_1n_2m_2} \mathcal{M}^{N'M'n'm'}_{n'_1m'_1n'_2m'_2} \\
&\cdot \int \text{đ}^2Q\,\text{đ}^2q\,\text{đ}^2Q'\,\text{đ}^2q'\, \frac{(2\pi)^2\delta^2(\sqrt{X}\boldsymbol{Q} - \sqrt{X'}\boldsymbol{Q}')}{D(\boldsymbol{q}, \boldsymbol{q}', \boldsymbol{Q} - \boldsymbol{Q}')} \Psi^M_N(Q)\Psi^m_n(q)\Psi^{M'*}_{N'}(Q')\Psi^{m'*}_{n'}(q')
\end{aligned} \tag{36}$$

Note that $X = X'$, hence $\boldsymbol{Q} = \boldsymbol{Q}'$, $D = D(\boldsymbol{q}, \boldsymbol{q}')$. In fact it is easy to show $\boldsymbol{k} = \frac{1}{\sqrt{X}}(\sqrt{x'_1x_2}\boldsymbol{q} - \sqrt{x_1x'_2}\boldsymbol{q}')$. So,

$$\begin{aligned}
I = &\sum_{NMnm} \sum_{N'M'n'm'} \mathcal{M}^{NMnm}_{n_1m_1n_2m_2} \mathcal{M}^{N'M'n'm'}_{n'_1m'_1n'_2m'_2} \delta_{N,N'}\delta_{M,M'} \\
&\cdot \int \text{đ}^2q\,\text{đ}^2q'\, \frac{1}{-\frac{(\sqrt{x'_1x_2}\boldsymbol{q} - \sqrt{x_1x'_2}\boldsymbol{q}')^2}{x_1-x'_1} + \frac{m_f^2X}{x_1} - \frac{m_f^2X}{x'_1} - \frac{\mu^2X}{x_1-x'_1}} \Psi^m_n(q)\Psi^{m'*}_{n'}(q')
\end{aligned}$$

Finally, we introduce "CM" and "relative" coordinates

$$\begin{aligned}
\boldsymbol{P} &\equiv \frac{\sqrt{x_1x'_2}\boldsymbol{q} + \sqrt{x'_1x_2}\boldsymbol{q}'}{\sqrt{x_1x'_2 + x'_1x_2}} \\
\boldsymbol{p} &\equiv \frac{\sqrt{x'_1x_2}\boldsymbol{q} - \sqrt{x_1x'_2}\boldsymbol{q}'}{\sqrt{x_1x'_2 + x'_1x_2}}
\end{aligned}$$

and do TM transform to the new coordinates,

$$
\begin{aligned}
I = &\sum_{NMnm} \sum_{N'M'n'm'} \sum_{N''M''n''m''} \mathcal{M}^{NMnm}_{n_1m_1n_2m_2} \mathcal{M}^{N'M'n'm'}_{n_1'm_1'n_2'm_2'} \mathcal{M}^{N'',M'',n'',m''}_{n,m,n',-m'} \delta_{N,N'}\delta_{M,M'} \\
&\cdot \int \text{đ}^2 P\, \Psi^{M''}_{N''}(P) \int \text{đ}^2 p\, \frac{1}{-\frac{x_1x_2'+x_1'x_2}{x_1-x_1'}\boldsymbol{p}^2 + (x_1+x_2)\left(\frac{m_f^2}{x_1} - \frac{m_f^2}{x_1'} - \frac{\mu^2}{x_1-x_1'}\right)} \Psi^{m''}_{n''}(p)
\end{aligned} \tag{37}
$$

The phases for each TM transform are $\delta = \arctan\sqrt{\frac{x_2}{x_1}}$, $\delta' = \arctan\sqrt{\frac{x_2'}{x_1'}}$, $\delta'' = \arctan\sqrt{\frac{x_1'x_2}{x_2'x_1}}$ respectively.

$$
I_n^m(\Delta) = \int \text{đ}^2 p\, \frac{1}{\boldsymbol{p}^2+\Delta} \Psi_n^m(p) = \frac{\delta_{m,0}}{\sqrt{4\pi}} \int \text{d}t \frac{1}{t+\Delta} e^{-t/2} L_n(t) \tag{38}
$$

where $L_n(t)$ is the Laguerre polynomial of the n-th order. Using the series expansion of Laguerre polynomials, the above expression can also be rewritten as,

$$
\begin{aligned}
I_n^m(\Delta) =&\delta_{m,0}\frac{e^{\Delta/2}}{\sqrt{4\pi}} \sum_{k=0}^{n} \binom{n}{k} (-1)^k \Delta^k \Gamma\left(-k, \frac{\Delta}{2}\right) \\
=&\delta_{m,0}\frac{e^{\Delta/2}}{\sqrt{4\pi}} \int_{\frac{\Delta}{2}}^{\infty} \text{d}t\, e^{-t} \left(1-\frac{\Delta}{t}\right)^n \frac{1}{t}
\end{aligned} \tag{39}
$$

where, $\Gamma(s,z) = \int_z^\infty \text{d}t\; e^{-t}t^{s-1}$ is the incomplete gamma function. Therefore, the energy denominator integral is,

$$
\begin{aligned}
I = &\delta_{m_1+m_2,m_1'+m_2'} \frac{x_1'-x_1}{x_1x_2'+x_1'x_2} \frac{e^{\Delta/2}}{2\pi} \sum_{m=\frac{m_1+m_2-\varepsilon}{2}}^{\frac{m_1+m_2+\varepsilon}{2}} \sum_{N=0}^{\min\{\mu,\nu\}} \sum_{N''=0}^{\mu+\nu+|m|-2N} \sum_{k=0}^{n''} \binom{n''}{k} (-1)^{k+N''} \\
&\cdot \mathcal{M}^{N,m_1+m_2-m,\mu-N,m}_{n_1,m_1,n_2,m_2} \mathcal{M}^{N,m_1'+m_2'-m,\nu-N,m}_{n_1',m_1',n_2',m_2'} \mathcal{M}^{N'',0,n'',0}_{\mu-N,m,\nu-N,-m} \Delta^k \Gamma\left(-k, \tfrac{\Delta}{2}\right)
\end{aligned} \tag{40}
$$

where, $E = 2(n_1+n_2)+|m_1|+|m_2|$, $E' = 2(n_1'+n_2')+|m_1'|+|m_2'|$, $\varepsilon = \min\{E, E'\}$, $\mu = (E-|m_1+m_2-m|-|m|)/2$, $\nu = (E'-|m_1'+m_2'-m|-|m|)/2$, $n'' = \mu+\nu+|m|-2N-N''$. $\Delta = \frac{x_1+x_2}{x_1x_2'+x_2x_1'}\left(m_f^2\frac{(x_1-x_1')^2}{x_1x_1'} - \mu^2\right)$.

6 The Longitudinal Confining Potential

The mass term in the kinetic energy is $\sum_a \frac{m_a^2}{x_a}$. For the tow-body system, Głazek et al [9] introduces a new longitudinal momentum $q_3 \equiv \frac{x_1m_2-x_2m_1}{\sqrt{x_1x_2}}$. The mass term can be rewritten as $\sum_a \frac{m_a^2}{x_a} = (m_1+m_2)^2 + q_3^2$. The newly introduced q_3 can be put into equal footing with $\boldsymbol{q}$, $\vec{q} = (\boldsymbol{q}, q_3)$. Similarly, the effective confining potential $\mathcal{V}_{\text{eff}}$ becomes a function of $\vec{s} = (\boldsymbol{s}, s_3)$, where $s_3 = \text{i}\partial_{q_3}$ is the conjugate coordinate of q_3. In the case of the soft-wall confining potential [2], this is equivalent to an additional longitudinal confining term $\kappa^4 s_3^2$. In our quarkonium application, $m_1 = m_2 = m_f$, $x_1 = x, x_2 = 1-x$, $q_3 = \frac{m_f(2x-1)}{\sqrt{x(1-x)}}$. Note that $\vec{q}$, $\vec{s}$ are not canonical variables. That's because $\left[s_3,\ \boldsymbol{q}\right] \neq 0$.

Recall $p^\mu x_\mu = p^+x_+ + p_+x^+ + p_ix^i$. Therefore, x_+ is the conjugate coordinate of p^+ and $[\hat{x}_+, \hat{p}^+] = \text{i}$. The momentum fraction $\hat{x} = \frac{\hat{p}^+}{P^+}$. Define $\hat{y} \equiv P^+\hat{x}_+$. Then $[\hat{y}, \hat{x}] = \text{i}$. So y is the conjugate coordinate of x and $y = \text{i}\partial_x$. In the DLCQ/BLFQ basis, $P^+ = \frac{2\pi}{L}K_{\max}$, $-\frac{1}{2}L \le x_+ \le +\frac{1}{2}L$, implying $-\pi K_{\max} \le y \le \pi K_{\max}$. Naïvely, we can define $s_3 = \frac{2}{m_f}(x(1-x))^{\frac{3}{2}}\text{i}\hat{y}$. But this operator is not Hermitian. A simple prescription is to symmetrize the operator:

$$
\hat{s}_3 = m_f^{-1}\left[(\hat{x}(1-\hat{x}))^{\frac{3}{2}}\hat{y} + \hat{y}(\hat{x}(1-\hat{x}))^{\frac{3}{2}}\right] \tag{41}
$$

It is easy to show $\left[(\hat{x}(1-\hat{x}))^{\frac{3}{2}}\hat{y},\ \frac{2\hat{x}-1}{\sqrt{\hat{x}(1-\hat{x})}}\right] = \frac{\text{i}}{2}$; $\left[\hat{y}(\hat{x}(1-\hat{x}))^{\frac{3}{2}},\ \frac{2\hat{x}-1}{\sqrt{\hat{x}(1-\hat{x})}}\right] = \frac{\text{i}}{2}$. Therefore, $\left[\hat{s}_3,\ \hat{q}_3\right] = i$.

$$
\hat{s}_3^2 = m_f^{-2}\left(\hat{\beta}\hat{y}\hat{\beta}\hat{y} + \hat{\beta}\hat{y}^2\hat{\beta} + \hat{y}\hat{\beta}^2\hat{y} + \hat{y}\hat{\beta}\hat{y}\hat{\beta}\right) \tag{42}
$$

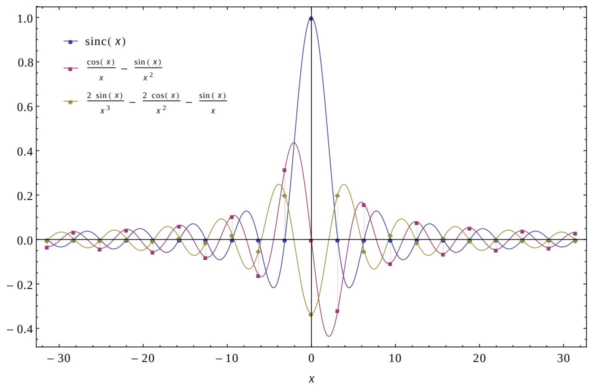


Figure 2: The plot of function sinc x and its first and second derivatives.

where $\hat{\beta} = \hat{x}(1-\hat{x}))^{\frac{3}{2}}$.

The matrix elements within the longitudinal plane-wave basis are,

$$\begin{aligned} m_f^2 \langle x'|\hat{s}_3^2|x\rangle =& 4(x'(1-x')x(1-x))^{\frac{3}{2}} \langle x'|\hat{y}^2|x\rangle \\ &+3\mathrm{i}(xx'(1-x)(1-x'))^{\frac{1}{2}}(x-x')((1-x)(1-x')+xx')\langle x'|\hat{y}|x\rangle \\ &+\tfrac{9}{4}(1-2x)^2x(1-x)\delta_{xx'}. \end{aligned} \tag{43}$$

In the DLCQ/BLFQ basis $\langle x|y\rangle = \mathscr{N} e^{\mathrm{i}xy}$. The normalization factor $\mathscr{N}$ can be determined from the orthonormal relation $\langle x'|x\rangle = \delta_{x'x}$:

$$\delta_{x'x} = \langle x'|x\rangle = \mathscr{N}^2 \int_{-\pi K_{\max}}^{+\pi K_{\max}} \mathrm{d}y \exp\left[\mathrm{i}y(x'-x)\right] = 2\pi K_{\max}\mathscr{N}^2 \mathrm{sinc}(\pi K_{\max}(x-x')) \tag{44}$$

where $\mathrm{sinc}\, x = \begin{cases} \frac{\sin x}{x} & x \neq 0 \\ 1 & x = 0. \end{cases}$ $\mathrm{sinc}[\pi K_{\max}(x-x')] = \delta_{xx'}$. Therefore, $\mathscr{N} = \frac{1}{\sqrt{2\pi K_{\max}}}$. Note that, $|y\rangle$ is not orthonormalized:

$$\langle y'|y\rangle = \sum_x \langle y'|x\rangle\langle x|y\rangle = \frac{1}{2\pi K_{\max}} \sum_{n=0}^{K_{\max}-1} \exp\left[\mathrm{i}(y-y')\frac{n+\frac{1}{2}}{K_{\max}}\right] = \frac{\exp\left[\frac{\mathrm{i}}{2}(y-y')\right]}{2\pi K_{\max}} \frac{\sin\frac{1}{2}(y-y')}{\sin\frac{(y-y')}{2K_{\max}}} \tag{45}$$

In the continuum limit $K_{\max} \to \infty$, $\langle y'|y\rangle \to \frac{1}{2}\delta(y-y')$.

$$\begin{aligned} \langle x'|\hat{y}|x\rangle &= \frac{1}{2\pi K_{\max}} \int_{-\pi K_{\max}}^{+\pi K_{\max}} \mathrm{d}y\; y \exp\left[-\mathrm{i}y(x-x')\right] = \mathrm{i}\partial_x \langle x'|x\rangle \\ &= \mathrm{i}\pi K_{\max}\left[\frac{\cos[\pi K_{\max}(x-x')]}{\pi K_{\max}(x-x')} - \frac{\mathrm{sinc}[\pi K_{\max}(x-x')]}{\pi K_{\max}(x-x')}\right]_{\mathrm{P.V.}} \end{aligned} \tag{46}$$

$$\begin{aligned} \langle x'|\hat{y}^2|x\rangle &= \frac{1}{2\pi K_{\max}} \int_{-\pi K_{\max}}^{+\pi K_{\max}} \mathrm{d}y\; y^2 \exp\left[-\mathrm{i}y(x-x')\right] = -\partial_x^2 \langle x'|x\rangle \\ &= \pi^2 K_{\max}^2 \left[\left(1 - \frac{2}{\pi^2 K_{\max}^2 (x-x')^2}\right)\mathrm{sinc}[\pi K_{\max}(x-x')] + \frac{2\cos[\pi K_{\max}(x-x')]}{\pi^2 K_{\max}^2 (x-x')^2}\right]_{\mathrm{P.V.}} \end{aligned} \tag{47}$$

Note that by invoking the Cauchy principle value, $\langle x|\hat{y}|x\rangle = 0$, $\langle x|\hat{y}^2|x\rangle = \frac{1}{3}\pi^2 K_{\max}^2$. The matrix element can also be computed directly from approximating the derivative by finite difference (See Fig. (3)). In general, the n-point finite difference can be obtained from the Lagrange interpolation,

$$\begin{aligned} f'(x) &= \sum_{k=1}^{n} \frac{(-1)^{k-1}(n)_k}{(n+1)^{(k)}} \frac{f(x+kh)-f(x-kh)}{kh} + \mathcal{O}(h^n) \\ f''(x) &= 2\sum_{k=1}^{n} \frac{(-1)^{k-1}(n)_k}{(n+1)^{(k)}} \frac{f(x+kh)+f(x-kh)-2f(x)}{k^2h^2} + \mathcal{O}(h^n) \end{aligned} \tag{48}$$

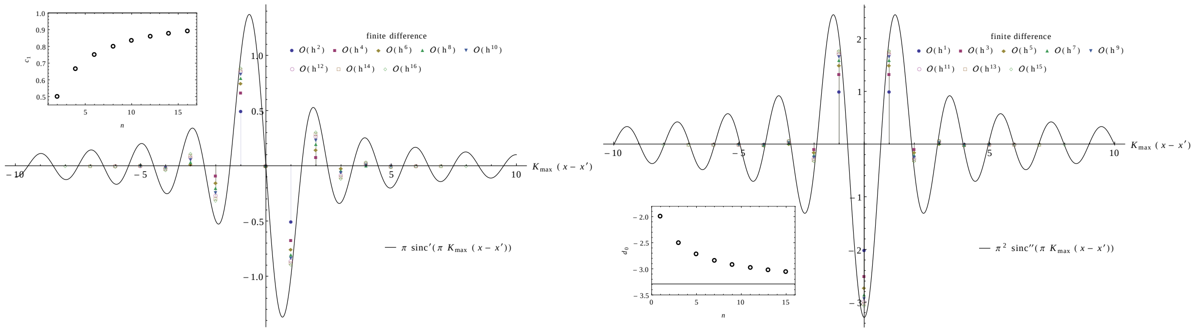


Figure 3: Comparison of two methods.

The leading order symmetric differences (3-point finite differences), for example, reads

$$\begin{aligned}&\partial_x \,|x\rangle \simeq \tfrac{1}{2}K_{\max}\left(|x+1/K_{\max}\,\rangle - |x-1/K_{\max}\,\rangle\right),\\ &\partial_x^2\,|x\rangle \simeq K_{\max}^2\left(|x+1/K_{\max}\,\rangle + |x-1/K_{\max}\,\rangle - 2\,|x\rangle\right).\end{aligned} \tag{49}$$

The following matrix elements are

$$\begin{aligned}&\langle x'|\mathrm{i}\partial_x|x\rangle \simeq \tfrac{\mathrm{i}}{2}K_{\max}\left(\delta_{x+\frac{1}{K_{\max}},x'} - \delta_{x-\frac{1}{K_{\max}},x'}\right),\\ &\left\langle x'|(\mathrm{i}\partial_x)^2|x\right\rangle \simeq K_{\max}^2\left(2\delta_{x,x'} - \delta_{x+\frac{1}{K_{\max}},x'} - \delta_{x-\frac{1}{K_{\max}},x'}\right).\end{aligned} \tag{50}$$

In this case, $\langle x|\mathrm{i}\partial_x|x\rangle = 0$, $\left\langle x|(\mathrm{i}\partial_x)^2|x\right\rangle = 2K_{\max}^2$.

Table 2: $\langle x'|\mathrm{i}\partial_x|x\rangle \simeq \mathrm{i}K_{\max}\cdot\sum_{k=-n}^{n} c_k\delta_{x+\frac{k}{K_{\max}},x'}$

n-point	$\delta_{x-\frac{3}{K_{\max}},x'}$	$\delta_{x-\frac{2}{K_{\max}},x'}$	$\delta_{x-\frac{1}{K_{\max}},x'}$	$\delta_{x,x'}$	$\delta_{x+\frac{1}{K_{\max}},x'}$	$\delta_{x+\frac{2}{K_{\max}},x'}$	$\delta_{x+\frac{3}{K_{\max}},x'}$
3-point			-1/2	0	+1/2		
5-point		1/12	-2/3	0	+2/3	-1/12	
7-point	-1/60	3/20	-3/4	0	+3/4	-3/20	+1/60

Table 3: $\left\langle x'|(\mathrm{i}\partial_x)^2|x\right\rangle \simeq K_{\max}^2\cdot\sum_{k=-n}^{n} c_k\delta_{x+\frac{k}{K_{\max}},x'}$

n-point	$\delta_{x-\frac{3}{K_{\max}},x'}$	$\delta_{x-\frac{2}{K_{\max}},x'}$	$\delta_{x-\frac{1}{K_{\max}},x'}$	$\delta_{x,x'}$	$\delta_{x+\frac{1}{K_{\max}},x'}$	$\delta_{x+\frac{2}{K_{\max}},x'}$	$\delta_{x+\frac{3}{K_{\max}},x'}$
3-point			-1	2	-1		
5-point		1/12	-4/3	5/2	-4/3	1/12	
7-point	-1/90	3/20	-3/2	49/18	-3/2	3/20	-1/90

In summary, the Fourier transform method gives,

$$\begin{aligned}m_f^2\left\langle x'|\hat{s}_3^2|x\right\rangle =&\,\delta_{xx'}x(1-x)\left[\tfrac{4\pi^2}{3}K_{\max}^2x^2(1-x)^2+\tfrac{9}{4}(1-2x)^2\right]\\ &+\delta_{x\neq x'}(-1)^{\Delta n}\sqrt{xx'(1-x)(1-x')}\left[\tfrac{8}{\Delta n^2}K_{\max}^2xx'(1-x)(1-x')-3(xx'+(1-x)(1-x'))\right],\end{aligned} \tag{51}$$

where $\Delta n = K_{\max}(x-x')$ is an integer.

The 3-point finite difference gives,

$$\begin{aligned}&m_f^2\left\langle x'|\hat{s}_3^2|x\right\rangle = \delta_{xx'}x(1-x)\left[8K_{\max}^2x^2(1-x)^2+\tfrac{9}{4}(1-2x)^2\right]\\ &-\delta_{|\Delta n|,1}\sqrt{xx'(1-x)(1-x')}\left[4K_{\max}^2xx'(1-x)(1-x')-\tfrac{3}{2}(xx'+(1-x)(1-x'))\right].\end{aligned} \tag{52}$$

The 5-point finite difference gives,

$$\begin{aligned} m_f^2 \langle x'|\hat{s}_3^2|x\rangle = \delta_{xx'} x(1-x) \left[10K_{\max}^2 x^2(1-x)^2 + \tfrac{9}{4}(1-2x)^2\right] \\ -\delta_{|\Delta n|,1}\sqrt{xx'(1-x)(1-x')}\left[\tfrac{16}{3}K_{\max}^2 xx'(1-x)(1-x') - 2(xx' + (1-x)(1-x'))\right] \\ +\delta_{|\Delta n|,2}\sqrt{xx'(1-x)(1-x')}\left[\tfrac{1}{3}K_{\max}^2 xx'(1-x)(1-x') - \tfrac{1}{2}(xx' + (1-x)(1-x'))\right]. \end{aligned} \tag{53}$$

The 7-point finite difference gives,

$$\begin{aligned} m_f^2 \langle x'|\hat{s}_3^2|x\rangle = \delta_{xx'} x(1-x) \left[\tfrac{98}{9}K_{\max}^2 x^2(1-x)^2 + \tfrac{9}{4}(1-2x)^2\right] \\ -\delta_{|\Delta n|,1}\sqrt{xx'(1-x)(1-x')}\left[6K_{\max}^2 xx'(1-x)(1-x') - \tfrac{9}{4}(xx' + (1-x)(1-x'))\right] \\ +\delta_{|\Delta n|,2}\sqrt{xx'(1-x)(1-x')}\left[\tfrac{3}{5}K_{\max}^2 xx'(1-x)(1-x') - \tfrac{9}{10}(xx' + (1-x)(1-x'))\right] \\ -\delta_{|\Delta n|,3}\sqrt{xx'(1-x)(1-x')}\left[\tfrac{2}{45}K_{\max}^2 xx'(1-x)(1-x') - \tfrac{3}{20}(xx' + (1-x)(1-x'))\right]. \end{aligned} \tag{54}$$

Note that as $\left[s_3, \boldsymbol{q}\right] \neq 0$, $\langle\, \boldsymbol{q}'|\hat{s}_3^2|\boldsymbol{q}\,\rangle \neq (2\pi)^2\delta^2(\boldsymbol{q}-\boldsymbol{q}')$. Recall $\left[s_3, \boldsymbol{p}\right] = 0$ and $|\boldsymbol{q}, x\rangle = \sqrt{x}\,|\boldsymbol{p}, x\rangle$. Therefore, $\langle\, \boldsymbol{q}', x'|\hat{s}_3^2|\boldsymbol{q}, x\,\rangle = \sqrt{xx'}(2\pi)^2\delta^2(\sqrt{x}\boldsymbol{q} - \sqrt{x'}\boldsymbol{q}')\,\langle\, x'|\hat{s}_3^2|x\,\rangle$. In the HO basis,

$$\begin{aligned} &\langle\, n'm'x'|\hat{s}_3^2|nmx\,\rangle = \int \text{đ}^2 q\,\text{đ}^2 q'\,\Psi_{n'}^{m'*}(\boldsymbol{q}')\Psi_n^m(\boldsymbol{q})\,\langle\, \boldsymbol{q}', x'|\hat{s}_3^2|\boldsymbol{q}, x\,\rangle \\ &= \int \text{đ}^2 q\,\text{đ}^2 q'\,\Psi_{n'}^{m'*}(\boldsymbol{q}')\Psi_n^m(\boldsymbol{q})\sqrt{xx'}(2\pi)^2\delta^2(\sqrt{x}\boldsymbol{q} - \sqrt{x'}\boldsymbol{q}')\,\langle\, x'|\hat{s}_3^2|x\,\rangle \\ &= \langle\, x'|\hat{s}_3^2|x\,\rangle\,\delta_{mm'}\left[\frac{2\sqrt{xx'}}{x+x'}\right]^{|m|+1}\sqrt{\frac{n!(n'+|m|)!}{n'!(n+|m|)!}}\left[\frac{x-x'}{x+x'}\right]^{n+n'}(-1)^{n'}\sum_{k=0}^{\min\{n,n'\}}\binom{n+|m|}{n-k}\binom{n'}{k}\frac{(-4xx')^k}{(x-x')^{2k}} \\ &\overset{\text{or}}{=} \langle\, x'|\hat{s}_3^2|x\,\rangle\,\delta_{mm'}(-1)^{n+n'}\frac{2\sqrt{xx'}}{x+x'}\sum_{N=0}^{n+n'+|m|}(-1)^N\,\mathcal{M}_{n,m,n',-m}^{N,0,n+n'-|m|,0}\Big|_{\delta=\arctan\sqrt{\frac{x'}{x}}} \end{aligned} \tag{55}$$

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