A complete set of Lorentz-invariant wave packets and modified uncertainty relation

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Abstract We define a set of fully Lorentz-invariant wave packets and show that it spans the corresponding one-particle Hilbert subspace, and hence the whole Fock space as well, with a manifestly Lorentz-invariant completeness relation (resolution of identity). The position–momentum uncertainty relation for this Lorentz-invariant wave packet deviates from the ordinary Heisenberg uncertainty principle, and reduces to it in the non-relativistic limit.

Contents

1 Introduction ...................................... 1
2 Gaussian basis and coherent states ............ 2
  2.1 Plane-wave basis ............................ 2
  2.2 Lorentz-friendly bases ..................... 4
  2.3 Gaussian basis .............................. 7
  2.4 Coherent states ............................. 8
3 Lorentz-invariant wave packet ............... 9
  3.1 Normalization .............................. 10
  3.2 Inner product .............................. 10
  3.3 Wave function .............................. 11
4 Uncertainty relations ............................ 13
  4.1 Momentum (co)variance ................... 13
  4.2 Position (co)variance ..................... 15
  4.3 Uncertainty relation ....................... 16
  4.4 Time–energy uncertainty ................. 16
5 Completeness of Lorentz-invariant basis ...... 17
6 Summary and discussion ....................... 18
Appendix A: More on coherent states  .......... 19
Appendix B: Master integral .................... 19
  B.1 Evaluation of master integral .......... 20
  B.2 Derivative of master integral .......... 21
  B.3 Integral of master integral .......... 21

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1 Introduction

Wave packets are one of the most fundamental building blocks of quantum field theory. We never observe a plane-wave state of, say, zero and infinite uncertainties of momentum and position, respectively. The plane-wave construction necessarily yields a square of the energy–momentum delta function in the probability, which hence is always divergent and is more a mnemonic than a derivation (quoted from Sect. 3.4 in textbook [1]).

However, so far, it has been widely believed that there are no intrinsically new phenomena appearing from a wave-packet construction, but recent developments imply that it might play important roles in vast areas of science; see e.g. the references in the Introduction in Ref. [2].

Up to now, the wave-packet S-matrix has been computed using a complete basis of Gaussian wave-packets; see e.g. Refs. [2–5]. The Gaussian basis is constructed from a Gaussian wave packet that evolves in time $t$ as $e^{-i\sqrt{m^2+p^2}t}$ for each plane-wave mode $p$, and is not manifestly Lorentz covariant nor invariant. To fully exploit the Lorentz covariance of S-matrix in quantum field theory, it is desirable to have a complete basis of Lorentz-invariant wave packets. This is what we propose in this paper.

Here we stress the viewpoint that the Gaussian basis is equivalent to a complete set of coherent states in the position–momentum phase space (see Refs. [6–10] and the references therein for works on coherent states in the context of the rel-

References ............................... 26

B.3.1 Saddle-point method ..................... 22
B.3.2 Non-relativistic expansion without using
saddle-point method ......................... 25
ativistic quantum mechanics\textsuperscript{1}). Guided by this equivalence, we develop the complete basis of Lorentz-invariant wave packets which is directly applicable in quantum field theory.

Our proposal is also inspired by the “relativistic Gaussian packet” \cite{16,17} developed by Naumov and Naumov (see also Refs. \cite{18–20}), and can be viewed as its generalization to form the complete set: From this viewpoint, our work can be interpreted as a new introduction of a spacetime center of wave packet as an independent variable, which is integrated over a spacelike hyperplane in the completeness relation along with a center of momentum.

It is worth mentioning that our Lorentz-invariant wave packet, when written in momentum space, is essentially the same as the one proposed in Refs. \cite{6,7}. What is new in relation along with a center of momentum is in agreement with that in Refs. \cite{6,7}, whereas the expectation value and uncertainty of the position on a constant time slice are obtained for the first time in this paper.

The organization of this paper is as follows: In Sect. 2, we review the plane-wave basis and the Gaussian basis, as well as the equivalence of the latter to the coherent basis, in order to spell out our notation. In Sect. 3, we present the Lorentz-invariant wave packet that we propose. In Sect. 4, we show some of the known facts on the coherent states. In Appendix B, we present detailed computations for integrals that we encounter in the main text.

2 Gaussian basis and coherent states

Here in order to spell out our notation, we review basic known facts about the plane-wave basis and the Gaussian one, as well as the equivalence of the latter to the coherent one in the position–momentum space.

\textsuperscript{1} It is well known that relativistic quantum mechanics is pathological and that quantum field theory is needed to remedy it; see e.g. Refs. \cite{11–15} and the references therein for related discussions; we clarify our standpoint in Sect. 2.

\textsuperscript{2} Throughout this paper, all the operators other than \( \hat{\phi}(x) \), \( \hat{\psi}(x) \), and \( \tilde{A}_\mu(x) \) are time-independent ones in the Schrödinger picture, unless otherwise stated.
We are focusing on the real scalar field in this paper because it is straightforward to generalize it to spinor and vector fields: We may expand these fields (in the interaction picture) as

\[
\hat{\psi}(x) = \sum_{s} \int \frac{d^d p}{(2\pi)^{d/2} \sqrt{2E_p}} \left( a_{p,s} e^{ip \cdot x} u(p, s) + a_{p,s}^\dagger e^{-ip \cdot x} v(p, s) \right),
\]

and may generalize the expressions below by the replacement \(a_p \rightarrow \hat{a}_{p,s}, \text{etc.}^3\)

Throughout this paper, we concentrate on the free one-particle Hilbert subspace \(L^2(\mathbb{R}^d)\) that is spanned by the free one-particle momentum basis in any physical experiment.

We stress that the Schrödinger-picture basis \(|x\rangle\) already specifies the particular frame \(x\) such that the Minkowski space is foliated by the constant-\(x^0\) spacelike hyperplanes and that the free one-particle Hilbert subspace is spanned on a Cauchy surface of a constant-\(x^0\) hyperplane, which we have chosen to be \(\Sigma(0)\). We also define, on each constant-\(x^0\) hyperplane \(\Sigma_{(x^0)}\) under this foliation, a “one-particle interaction basis” \(|x\rangle\) by

\[
\langle x | p \rangle := \frac{e^{ip \cdot x}}{(2\pi)^{d/2}}.
\]

Strictly speaking, \(|x\rangle\) should be regarded as spanning the space \(K_{(x^0)}\) of positive-energy solutions to the Klein–Gordon equation at \(x^0\), given the initial data \(L^2(\Sigma(0))\) on the Cauchy surface \(\Sigma(0)\), whereas one would expect that this is equivalent to \(L^2(\Sigma_{(x^0)})\) due to the time-translational invariance of the theory. Hereafter, we write \(L^2(\Sigma_{(x^0)})\) but the cautious reader may recast it into \(K_{(x^0)}\).

We can define the formal momentum operator \(\hat{p}\) on \(L^2(\mathbb{R}^d)\) by

\[
\hat{p} | p \rangle := p | p \rangle,
\]

and the formal position operator \(\hat{x}\) as the generator of momentum translation on \(L^2(\mathbb{R}^d)\) by\(^5\)

\[
\langle p | \hat{x} := i \nabla_p \langle p | ,
\]

on \(L^2(\Sigma(0))\), which is consistent with Eqs. (10) and (13). We note that \(\hat{x}\) and \(|x\rangle\) are the time-independent ones in the Schrödinger picture by construction; recall footnote 2.

Here we stress that the position and momentum bases \(|x\rangle\) and \(|p\rangle\) have infinite norms \(|x| x\rangle = \infty\) and \(|p | p\rangle = \infty\), respectively, so that they do not belong to \(L^2(\mathbb{R}^d)\) nor to \(L^2(\Sigma(0))\). We never realize \(|x\rangle\) nor \(|p\rangle\) in any physical experiment. The formal position and momentum operators \(\hat{x}\) and \(\hat{p}\)

\(^3\) If one would define the position basis as \(|x\rangle = \hat{\psi}^*(x) |0\rangle\), etc., the “Lorentz-invariant wave function” should read the “Lorentz-covariant wave function” accordingly. The position basis for the anti-particle should read \(|x, c\rangle = \hat{\psi}(x) |0\rangle\) in such a case.

\(^4\) Hereafter, “basis” is used as an abbreviation of a “basis vector” or “basis state” of a Hilbert space, and denotes a state that can be regarded as an eigenstate of an operator that has proper time evolution in a given picture: Namely, a basis evolves as \(|\phi\rangle, e^{iH_{tot} x^0} |\phi\rangle, e^{iH_{tot}} |\phi\rangle\) in the Schrödinger, interaction, and Heisenberg pictures, respectively, with \(H = H_{tot} + H_{int}\). For example, \(|p\rangle\) is a basis in the Schrödinger picture.

Later, we will call, say, \(|x\rangle\) the basis, even though it is not an eigenvector of a Hermitian operator but of a non-Hermitian one (43). See e.g. Refs. [21,22] for treatment of non-Hermitian operator.

\(^5\) As always, this is written as an operator relation that denotes, for any normalizable physical state \(|\psi\rangle\), \(\langle p | \hat{x} | \psi\rangle = i \nabla_p \langle p | \psi\rangle\). Strictly speaking, the eigenstates of \(\hat{x}\) and \(\hat{p}\) are not an element of \(L^2(\Sigma(0))\) and \(L^2(\mathbb{R}^d)\), respectively, hence the wording “formal”; see below for more discussion.
and their eigenbases $|x\rangle$ and $|p\rangle$, respectively, are mere mathematical tools to write down their expectation values basis-independently for any shape of normalizable wave packet $|\psi\rangle$ in $L^2(\Sigma_{(0)})$ or $L^2(\mathbb{R}^d)$ as

$$
\langle \hat{x}| \psi \rangle = \frac{1}{\langle \psi | \psi \rangle} \int d^3x |\psi(x)|^2 x_i
$$

$$
= \frac{1}{\langle \psi | \psi \rangle} \int d^3p \hat{p}^\dagger(p) \left(i \frac{\partial}{\partial p^i}\right) \psi(p), \quad (15)
$$

$$
\langle \hat{p}| \psi \rangle = \frac{1}{\langle \psi | \psi \rangle} \int d^3x \langle \psi(x) | -i \frac{\partial}{\partial x^i}\rangle \psi(x), \quad (16)
$$

where $\langle x | \psi \rangle = \langle \psi | x \rangle$, $\langle p | \psi \rangle = \langle \psi | p \rangle$, and $\langle \psi | \psi \rangle = \int d^3x |\psi(x)|^2 = \int d^3p |\psi(p)|^2 < \infty$. This fact of the non-normalizability of basis is indeed one of the motivations of the Gaussian construction and its Lorentz-invariant generalization presented in this paper.

The formal operator $\hat{x}$ is first defined as the generator of momentum translation (13), and is associated with a particular foliation of spacetime through Eq. (14) such that $\Sigma_{(0)}$ is chosen as the Fourier transform of the momentum space $\mathbb{R}^d$ via Eq. (10). Once this association with the position space is fixed, $\hat{x}$ is tied to the particular reference frame, with its unit spatial volume $d^3x$ manifestly violating the Lorentz invariance. The position operator $\hat{x}$ is not covariant by construction; see also Ref. [15] for a review on the Lorentz non-covariance from the point of view of relativistic quantum mechanics.

We may regard $\hat{p}$ as a restriction of the momentum operator (4) to the free one-particle subspace $L^2(\mathbb{R}^d)$: Schematicly,

$$
\hat{P}_{\text{free}} = \begin{bmatrix}
0 & 0 & 0 & \cdots \\
0 & \hat{p} & 0 & \cdots \\
0 & 0 & \ast & \cdots \\
\ldots & \ldots & \ldots & \ldots
\end{bmatrix},
\begin{bmatrix}
|0\rangle \\
|1\rangle \\
|2\rangle \\
\vdots
\end{bmatrix} = \begin{bmatrix}
\text{1-particle subspace} \\
\ast \\
\vdots
\end{bmatrix}. \quad (17)
$$

Similarly, when restricted to the one-particle subspace,

$$
\hat{H}_{\text{free}} := \hat{H}_{\text{free}} |_{L^2(\mathbb{R}^d)} = E\hat{p} = \sqrt{m^2 + \hat{p}^2}. \quad (18)
$$

It also follows that, on $L^2(\Sigma_{(0)})$,

$$
\langle x | \hat{p} | p \rangle = -i \nabla \langle x | p \rangle, \quad \langle \hat{p} | x \rangle = i \langle x | \nabla \rangle
$$

such that $\langle x | \hat{p} | p \rangle = -i \nabla \langle x | p \rangle = -i \nabla \frac{\langle p | x \rangle}{(2\pi)^d} = \frac{p}{(2\pi)^d} = p \langle x | p \rangle$, with $\nabla_i := \partial/\partial x^i$.

We may relate the bases of $L^2(\Sigma_{(0)})$ and $L^2(\Sigma_{(0)})$ by

$$
|\psi\rangle = e^{iE\hat{p}x^0} |x\rangle. \quad (20)
$$

The position operator $\hat{x}$ can be trivially extended to $L^2(\Sigma_{(0)})$:

$$
\hat{x} |\psi\rangle = \hat{x} e^{iE\hat{p}x^0} |x\rangle = \left(x - \frac{\hat{p}}{E\hat{p}}x^0\right) |x\rangle, \quad (21)
$$

where we used $[\hat{x}, \hat{p}] = i \frac{\partial}{\partial p^i}(\hat{p})$.

On $L^2(\Sigma_{(0)})$, the plane-wave normalization is

$$
|x| = \delta^d(x - x'). \quad (22)
$$

We may also formally write down the inner product of bases of $L^2(\Sigma_{(0)})$ and of $L^2(\Sigma_{(0)})$,

$$
\langle x | x' \rangle = \int d^dp \langle x | p \rangle \langle p | x' \rangle = \int \frac{d^dp}{(2\pi)^d} e^{ip(x-x')} = \int \frac{d^dp}{(2\pi)^d} e^{-iE\hat{p}(x''-x') + ip(x-x')}. \quad (23)
$$

The completeness relations on $L^2(\Sigma_{(0)})$ and on $L^2(\Sigma_{(0)})$ are, respectively,

$$
\int d^dx |x\rangle \langle x| = \hat{1}, \quad \int d^dx |x\rangle \langle x| = \hat{1}. \quad (24)
$$

The mass dimensions are $[|x|] = [|\psi|] = \frac{q}{2}$.

### 2.2 Lorentz-friendly bases

From here we start to deviate from the standard notation in the literature. Our so-called “Lorentz-friendly basis” is essentially the same as the basis proposed by Newton and Wigner [11], which was later complemented in terms of the Euclidean group by Wightman [12].

In Refs. [13,14] it has been shown that (so-called) “strict localization”, which requires a wave function $\psi(x) = |x| |\psi\rangle$ in $L^2(\Sigma_{(0)})$ to vanish everywhere outside a finite region $V \subset \Sigma_{(0)}$, cannot be consistent with what the authors call “causality”, which we will refer to as “Hegerfeldt causality”. Hegerfeldt causality holds when the following is satisfied: If $\psi$ is strictly localized to $V$, then there should exist $r$ that makes $|x| e^{-iH_{\text{free}}E\hat{p}\hat{x}^0} |\psi\rangle = 0$ for all $x \in V$ for all $a$ with $a > r$ at any later time $t^0 > 0$. The authors have proven that Hegerfeldt causality is necessarily violated [13,14]. From Eq. (22), the position basis $|x\rangle$, interpreted as a wave function of $x$ in $L^2(\Sigma_{(0)})$ (closing our eyes on the fact that it cannot the case due to its non-normalizability), is strictly localized. Therefore, it obeys the proven violation of Hegerfeldt causality. On the other hand, both the Gaussian wave packet (58) and our extension (104) have exponentially small but non-zero tail outside any finite region $V$ from the beginning on $\Sigma_{(0)}$ and later. Therefore, they evade the condition of strict localization of Hegerfeldt causality from the beginning.
We define a “Lorentz-friendly” annihilation operator on $\mathcal{H}$:

$$\hat{\alpha}_p = \sqrt{2E_p} \hat{\alpha}_0,$$

which gives

$$\left[\hat{\alpha}_p, \hat{\alpha}_p^\dagger\right] = 2E_p \delta^d(p - p') \hat{1}, \quad \text{others } = 0,$$

and

$$\hat{\phi}(x) = \int \frac{d^dp}{(2\pi)^d} \left( \hat{\alpha}_p e^{ip\cdot x} + \hat{\alpha}_p^\dagger e^{-ip\cdot x} \right) = \int \frac{d^dp}{(2\pi)^d} \delta(p^2 + m^2) \hat{\phi}(p) \left( \hat{\alpha}_p e^{ip\cdot x} + \hat{\alpha}_p^\dagger e^{-ip\cdot x} \right).$$

where the Lorentz invariance is made manifest in the last expression by letting $p$ be off-shell.

We define a Lorentz-friendly position basis that spans $L^2(\mathbb{R}^d)$:

$$|p\rangle := \hat{\alpha}_p |0\rangle = \sqrt{2E_p} |p\rangle$$

such that

$$\langle p | p'\rangle = 2E_p \delta^d(p - p'), \quad \int \frac{d^dp}{2E_p} |p\rangle \langle p| = \hat{1}. \quad (29)$$

Mass dimensions are $[\hat{\alpha}_p] = [|p\rangle] = -\frac{d-1}{2}$. This completeness is the same as Eq. (1) in Ref. [11] up to the factor 2 (which will not be mentioned hereafter).

We also define Lorentz-friendly position bases in $L^2(\Sigma_0)$ and in $L^2(\Sigma_{x,0})$, respectively:$^7$

$$|x\rangle := \hat{\phi}(x) |0\rangle = \int \frac{d^dp}{(2\pi)^d} \sqrt{2E_p} e^{-ip\cdot x} |p\rangle,$$

$$|x\rangle := \hat{\phi}(x) |0\rangle = \int \frac{d^dp}{(2\pi)^d} \sqrt{2E_p} e^{-ip\cdot x} |p\rangle.$$ (30)

The mass dimensions are $[|x\rangle] = [|x\rangle] = \frac{d-1}{2}$. Here, $|x\rangle$ and $|x\rangle$ are generalizations of the one-particle position bases in the Schrödinger and interaction pictures, respectively. They satisfy

$$\langle x | p\rangle = \frac{e^{ip\cdot x}}{(2\pi)^d} = \langle x | p\rangle, \quad \langle x | p\rangle = \frac{e^{ip\cdot x}}{(2\pi)^d} = \langle x | p\rangle.$$ (32)

Now we can write the field operator on $\mathcal{H}$ as

$$\hat{\phi}(x) = \int \frac{d^dp}{2E_p} \left( \langle x | p\rangle \hat{\alpha}_p + \hat{\alpha}_p^\dagger \langle p | x\rangle \right).$$ (33)

Note that a wave function $\langle x | \Phi \rangle$ is equivalent to the one given in Eq. (2) in Ref. [11].

On $L^2(\Sigma_0)$, we may formally write

$$\langle x | \rangle = \langle x | \frac{1}{\sqrt{2E_p}} \rangle = \frac{1}{\sqrt{2\sqrt{m^2 - \nabla^2} + m^2}} \langle x | \rangle.$$ (34)

The normalization on $L^2(\Sigma_{x,0})$ is

$$\langle x | x'\rangle = \int \frac{d^dp}{2E_p} \langle x | p\rangle \langle p | x'\rangle$$

$$= \int \frac{d^dp}{(2\pi)^d} e^{ip\cdot (x-x')}.$$ (35)

and we may again write down the inner product of bases of $L^2(\Sigma_{x,0})$ and of $L^2(\Sigma_{x,0})$: $^8$

$$\langle x | x'\rangle = \int \frac{d^dp}{2E_p} \langle x | p\rangle \langle p | x'\rangle$$

$$= \int \frac{d^dp}{(2\pi)^d} e^{ip\cdot (x-x')}.$$ (36)

On $L^2(\Sigma_0)$, the completeness relation becomes

$$\hat{1} = \int d^dx \sqrt{2E_p} \langle x | \langle x | \sqrt{2E_p}$$

$$= \int d^dx \left[ \langle x | \sqrt{2\sqrt{m^2 - \nabla^2} + m^2} \langle x | \right]$$

$$= \int d^dx 2E_p \langle x | \rangle \langle x |$$

$$= \int d^dx \left[ \langle x | 2\sqrt{m^2 - \nabla^2} \langle x | \right]$$

$$= \int d^dx \langle x | 2E_p$$

$^7$ See footnote 4.

$^8$ From this, the Feynman propagator is given by

$$D_F(x-x') = \theta(x_0 - x'_0) \{x | x'\} + \theta(x_0 - x'_0) \{x' | x\}$$

$$= \int \frac{d^dP}{(2\pi)^d} e^{iP\cdot (x-x')} \frac{-i}{P^2 + m^2 - i\epsilon}.$$ (37)

One may find its explicit form as a function of $(x-x')^2$ c.g. in Ref. [23].
which can be checked by sandwiching the two sides by \( \langle \langle p \rangle \rangle \) and \( \langle \langle \hat{p} \rangle \rangle \). The same relation holds on \( L^2(\Sigma_{E(0)}) \) when we replace \( |x\rangle \) and \( \langle x| \) by \( \langle \langle x| \rangle \rangle \) and \( \langle \langle x| \rangle \rangle \), respectively, because the factors \( e^{-i\sqrt{m^2 + \nabla^2}x^0} \) cancel out each other. Now we may rewrite the above completeness relation in a manifestly Lorentz-invariant fashion\(^9\) on an arbitrary \( L^2(\Sigma) \) space, with the same precaution as given after Eq. (11):

\[
\hat{1} = \int \frac{d^d \Sigma^\mu}{\Sigma} \left[ 2i \frac{\partial}{\partial x^\mu} \langle \langle x| \rangle \rangle \right] = \int \frac{d^d \Sigma^\mu}{\Sigma} \left[ \langle x| \rangle \left( -2i \frac{\partial}{\partial x^\mu} \right) \langle \langle x| \rangle \rangle \right],
\]

where \( d^d \Sigma^\mu \) is the surface element normal to \( \Sigma \). (In the language of differential forms, it is nothing but the induced volume element \( d^d \Sigma^\mu = -d^d x^\mu \), with \( * \) denoting the Hodge dual; in flat spacetime, we get \( d^d x^\mu = \frac{1}{n!} \epsilon^{\mu_\nu_{\lambda_1} \cdots \lambda_{n-1}} dx_\lambda \wedge \cdots \wedge dx_\lambda \) with \( \epsilon_{01 \cdots d} = 1 \).

Physically, a probability density \( P(x) \) (per unit volume \( d^d x \)) of observing the particle at a position \( x \) at time \( x^0 \) for a (normalized) wave packet \( |\psi\rangle \) is given by the expectation value of the projector \( |x\rangle \langle x| \) on \( L^2(\Sigma_{E(0)}) \):\(^10\)

\[
P(x) = \langle \psi | x \rangle \langle x | \psi \rangle = \langle \psi | \sqrt{2E_p} | x \rangle \langle x | \sqrt{2E_p} | \psi \rangle = \left| \frac{1}{2\sqrt{m^2 - \nabla^2}} \langle x | \psi \rangle \right|^2.
\]

Note that the probability density is not merely the absolute-square of the wave function.

The following relations on \( L^2(\mathbb{R}^d) \) may be useful:

\[
\langle \langle p| \hat{x} \rangle \rangle = \sqrt{2E_p} i \nabla_p \langle \langle p| \rangle \rangle = i \nabla_p \langle \langle p| \rangle \rangle - i \frac{p}{2E_p} \langle \langle p| \rangle \rangle
\]

and we get

\[
\langle \langle x| \hat{x} \rangle \rangle = \left( \frac{x - i \frac{\hat{p}}{2E_p} x^0}{\sqrt{2E_p}} \right) \langle \langle x| \rangle \rangle
\]

\[
\langle \langle x| \hat{\nabla} \rangle \rangle = \left( \frac{x - \frac{\hat{p}}{E_p} x^0 - i \frac{\hat{p}}{2E_p}}{\sqrt{2E_p}} \right) \langle \langle x| \rangle \rangle.
\]

The wave function is of the form \( e^{-iH_{free}^\mu \cdot e^{-iH_{int}^\mu} |\psi\rangle} \) with \( H = H_{free} + H_{int} \). Throughout this paper, we neglect interactions, \( H_{int} = 0 \), and hence it suffices to treat the time dependence as in the main text.

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\( ^9 \) More precisely, the relation becomes Lorentz invariant when the two sides are sandwiched by the basis states \( \langle \langle p| \rangle \rangle \) and \( \langle \langle q| \rangle \rangle \).

\( ^10 \) We are working in the interaction picture and hence the time dependence of the wave function is of the form \( e^{iH_{free}^\mu \cdot e^{-iH_{int}^\mu} |\psi\rangle} \) with \( H = H_{free} + H_{int} \). Throughout this paper, we neglect interactions, \( H_{int} = 0 \), and hence it suffices to treat the time dependence as in the main text.

---

Table 1: Eigenvalues of \( \hat{p} \) and \( \hat{x} \) or \( \hat{\chi} \) on various states

| State | \( \hat{p} \) | \( \hat{x} = \hat{x} - i \frac{\hat{p}}{2E_p} \) |
|-------|----------------|-----------------|
| \( \langle \langle p| \hat{p} \rangle \rangle \) | \( \langle \langle p| \hat{p} \rangle \rangle \) | \( \langle \langle p| \hat{p} \rangle \rangle \) |
| \( \langle \langle x| \hat{p} \rangle \rangle \) | \( \langle \langle x| \hat{p} \rangle \rangle \) | \( \langle \langle x| \hat{p} \rangle \rangle \) |
| \( \langle \langle x|e^{-iE_p x^0} \hat{p} \rangle \rangle \) | \( \langle \langle x|e^{-iE_p x^0} \hat{p} \rangle \rangle \) | \( \langle \langle x|e^{-iE_p x^0} \hat{p} \rangle \rangle \) |
| \( \langle \langle p| = \sqrt{2E_p} \langle \langle p| \hat{p} \rangle \rangle \) | \( \langle \langle p| \hat{p} \rangle \rangle \) | \( \langle \langle p| \hat{p} \rangle \rangle \) |
| \( \langle \langle x| = \langle \langle x| \hat{p} \rangle \rangle \) | \( \langle \langle x| \hat{p} \rangle \rangle \) | \( \langle \langle x| \hat{p} \rangle \rangle \) |
| \( \langle \langle x| = \langle \langle x|e^{-iE_p x^0} \hat{p} \rangle \rangle \) | \( \langle \langle x|e^{-iE_p x^0} \hat{p} \rangle \rangle \) | \( \langle \langle x|e^{-iE_p x^0} \hat{p} \rangle \rangle \) |

In each set of three rows separated by the horizontal lines, the first, second, and third rows are given in the Hilbert spaces \( L^2(\mathbb{R}^d) \), \( L^2(\Sigma_{E(0)}) \), and \( L^2(\Sigma_{E(0)}) \), respectively.

Equation (40) is equivalent to Eq. (11) in Ref. [11] up to the metric sign convention.

We may formally define non-Hermitian position-like operator:\(^11\)

\[
\hat{\chi} := \sqrt{2E_p} \hat{\nabla} \frac{1}{\sqrt{2E_p}} \hat{x} - i \frac{\hat{p}}{2E_p},
\]

which satisfies

\[
\langle \langle x| \hat{\chi} \rangle \rangle = \langle \langle x| \hat{\nabla} \rangle \rangle \langle \langle x| \hat{x} \rangle \rangle = x \langle \langle x| \rangle \rangle,
\]

\[
\langle \langle p| \hat{\chi} \rangle \rangle = i \nabla_p \langle \langle p| \rangle \rangle = \langle \langle p| \hat{\nabla} \rangle \rangle \langle \langle p| \rangle \rangle = \langle \langle p| \hat{\nabla} \rangle \rangle \langle \langle p| \rangle \rangle = \langle \langle p| \hat{\chi} \rangle \rangle \langle \langle p| \rangle \rangle.
\]

on \( L^2(\Sigma_{E(0)}) \) and on \( L^2(\mathbb{R}^d) \), respectively. Note that e.g. \( |x\rangle \) is not an eigenbasis of \( \hat{\chi} \) but of \( \hat{\chi}^\dagger \). In Eq. (44), the eigenvalues happen to be real for the non-Hermitian operators \( \hat{\chi} \) and \( \hat{\chi}^\dagger \), respectively.

We summarize the results for various bases in Table 1.

Finally, we comment on the Lorentz-transformation property of the one-particle momentum and position operators on

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\( ^11 \) This operator has been discussed in Ref. [19] and references therein, where \( \hat{\chi} \) is treated as self-adjoint. Our claim differs in that \( \hat{\chi} \) is manifestly non-self-adjoint.
From Eqs. (31) and (51), we see that \( \chi \) which yields \( \chi \) again, reinterpreting this as transformation on operators \( \hat{p}^i \) which yields \( \hat{p}^i | p \rangle = (\Lambda p)^i | p \rangle \).

The momentum operator is covariant on \( L^2(\mathbb{R}^d) \) in this sense. The transformation (47) yields

\[
\tilde{\phi}(x) \to \hat{U}_{\text{free}}(\Lambda, b) \tilde{\phi}(x) \hat{U}^\dagger_{\text{free}}(\Lambda, b) = \hat{\phi}(\Lambda x + b) \quad \text{(51)}
\]

From Eqs. (31) and (51), we see that

\[
| x \rangle \to \hat{U}_{\text{free}}(\Lambda, b) | x \rangle = | \Lambda x + b \rangle \quad \text{(52)}
\]

Again, reinterpreting this as transformation on operators

\[
\hat{x}^{i\dagger} \to \hat{x}_{\Lambda,b}^{i\dagger} := \hat{U}^\dagger_{\text{free}}(\Lambda, b) \hat{x}^{i\dagger} \hat{U}_{\text{free}}(\Lambda, b) \quad \text{(53)}
\]

We can show that

\[
\hat{x}_{\Lambda,b}^{i\dagger} | x \rangle = (\Lambda x + b)^i | x \rangle \quad \text{(54)}
\]

We see that, on the Lorentz-friendly basis \( | x \rangle \) in \( L^2(\Sigma_{(x_0)}) \), the non-Hermitian operator \( \hat{x}^{i\dagger} \) is the spatial component of a Poincaré-covariant vector. On the other hand, we clearly see that the physical position operator \( \hat{x} = \hat{x}^{i\dagger} - i \frac{\hat{p}^i}{2E} \) is not a spatial component of a Lorentz-covariant vector due to the second term. From the point of view of modern quantum field theory, it is not compulsory that \( \hat{x} \), associated to a particular spacetime foliation \( \Sigma_{(x_0)} \), with time slices of constant \( x_0 \), be a covariant operator. Of course, the whole theory is Lorentz invariant in the sense that the S-matrix, constructed from the covariant quantum fields (51) defined in the whole space \( \mathcal{H} \), is Lorentz invariant.

### 2.3 Gaussian basis

We define the Gaussian basis states through a normalizable, hence physical, wave function on \( L^2(\mathbb{R}^d) \) [3]:

\[
| \sigma; X, P \rangle := \left( \frac{\sigma}{\pi} \right)^{\frac{d}{4}} e^{\frac{1}{\sigma}(\sigma \cdot P - \sqrt{\sigma} P \cdot x)^2} \quad \text{(55)}
\]

\[
| \sigma; X, P \rangle := \left( \frac{\sigma}{\pi} \right)^{\frac{d}{4}} e^{\frac{1}{\sigma}(\sigma \cdot P - \sqrt{\sigma} P \cdot x)^2} \quad \text{(56)}
\]

where \( X \) and \( P \) are the centers of position and momentum of the wave packet, respectively, at time \( x_0 = 0 \) for Eq. (55) and \( x_0 = X^0 \) for (56), while \( \sigma > 0 \) is its width-squared. We see that these states on \( L^2(\mathbb{R}^d) \) are related by

\[
| \sigma; X, P \rangle = e^{iE_\sigma x^0} | \sigma; X, P \rangle \quad \text{(57)}
\]

Due to this dependence on \( X^0 \), one might want to regard the physical states \( | \sigma; X, P \rangle \) and \( | \sigma; X, P \rangle \) as some bases in the Schrödinger and interaction pictures on \( L^2(\Sigma_{(x)}) \) and \( L^2(\Sigma_{(x_0)}) \), respectively, through the Fourier transformation. However, when we consider the wave function (59) below, \( X^0 \) is rather a parameter that specifies the shape of the wave packet, and the time coordinate is \( x^0 \).

Again through the Fourier transformation, we may map the momentum-space wave functions onto \( L^2(\Sigma_{(0)}) \) and \( L^2(\Sigma_{(x_0)}) \):

\[
\langle x | \sigma; X, P \rangle = \int d^d p \langle x | p \rangle \langle p | \sigma; X, P \rangle = \int d^d p \langle x | p \rangle \langle p | \sigma; X, P \rangle = \frac{1}{(2\pi)^\frac{d}{2}} \int d^d p e^{i\rho (x^0 - X^0)} e^{-\frac{\rho}{2} (p \cdot x - x_0)^2} \quad \text{(58)}
\]

\[
\langle x | \sigma; X, P \rangle = \frac{1}{(2\pi)^\frac{d}{2}} \int d^d p e^{i\rho (x^0 - X^0)} e^{-\frac{\rho}{2} (p \cdot x - x_0)^2} \quad \text{(59)}
\]

At the leading saddle-point approximation for large \( \sigma \), Eq. (59) reduces to a closed form [4]:

\[
\langle x | \sigma; X, P \rangle \to \left( \frac{1}{\pi \sigma} \right)^{d/4} \frac{1}{\sqrt{2p_0}} e^{p_0(x - x)(x - x - V(x - x_0)^2)} \quad \text{(60)}
\]

\[\text{Footnotes:}
\]

12 Here we only consider orthochronous \( \Lambda \) so that \( \hat{U}_{\text{free}}(\Lambda, b) \) is linear and unitary.

13 See also footnotes 4 and 5.
where $P$ is on-shell $P^0 = E_P$ as always, and we define $V := P/P^0$. We see that the center of the wave packet moves as $X + V (x^0 - X^0)$ when we vary time $x^0$, namely, when we change the time-slice $\Sigma(x^0)$.

The inner product in $L^2(\mathbb{R}^d)$ is not orthogonal:

$$
\langle \sigma; X, P \mid \sigma'; X', P' \rangle = 
\left( \frac{\sigma_1}{\sigma_\Lambda} \right)^{\frac{d}{2}} e^{-\frac{1}{2\sigma^2}(X-X')^2} e^{-\frac{1}{2}(P-P')^2} e^{\sigma P \cdot \sigma' P'} \langle X-X' \rangle,
$$

where $\sigma_\Lambda := \frac{\sigma + \sigma'}{2}$ and $\sigma_1 := \left( \frac{\sigma^{-1} + \sigma'^{-1}}{2} \right)^{-1} = \frac{2\sigma\sigma'}{\sigma + \sigma'} = \frac{\sigma_\Lambda}{\sigma_1}$ are the average and the inverse of the average, respectively [5].

It is important that the Gaussian basis, with any fixed $\sigma$, form an (over)complete set in the free one-particle subspace $L^2(\mathbb{R}^d)$, $\sigma$.

$$
\int \frac{d^dX d^dP}{(2\pi)^d} |\sigma; X, P \rangle \langle \sigma; X, P | = I.
$$

Because any fixed $\sigma$ suffices to provide the complete set spanning $L^2(\mathbb{R}^d)$, we omit the label $\sigma$ usually. We may expand any wave function (or field configuration obeying the Klein–Gordon equation) $\psi(x) = \langle x | \psi \rangle$ by the Gaussian complete set $\{|X, P \rangle \}_X, P$ that spans $L^2(\mathbb{R}^d)$:

$$
\psi(x) = \int \frac{d^dX d^dP}{(2\pi)^d} \langle X, P \rangle \langle X, P | \psi \rangle.
$$

and conversely, the expansion coefficient may be computed by

$$
\langle X, P | \psi \rangle = \int d^dX \langle X, P | x \rangle \langle x | \psi \rangle
= \frac{1}{(\pi \sigma)^{\frac{d}{2}}} \int d^dX e^{-\frac{1}{2\sigma}(x-X)^2} \langle x | \psi \rangle
= \int d^dP \langle X, P | p \rangle \langle p | \psi \rangle
= \left( \frac{\sigma}{\pi} \right)^{\frac{d}{4}} \int d^dP e^{iPX} e^{-\frac{1}{2}(P-P')^2} \langle p | \psi \rangle.
$$

2.4 Coherent states

Here we see that a Gaussian wave packet is indeed a coherent state [24, 25] in the free-one-particle subspace $L^2(\mathbb{R}^d)$, or equivalently in $L^2(\Sigma_{(0)})$.

We define an “annihilation” operator for a $d$-dimensional harmonic oscillator:

$$
\hat{a} := \lambda \left( \frac{\hat{x}}{\sqrt{\sigma}} + i\sqrt{\sigma} \hat{p} \right), \quad \hat{a}^\dagger := \lambda^* \left( \frac{\hat{x}}{\sqrt{\sigma}} - i\sqrt{\sigma} \hat{p} \right),
$$

where $\lambda$ is an overall normalization, which is usually taken to be $\lambda = 1/\sqrt{2}$ but we leave it as an arbitrary complex number here. (More specifically, $\hat{p}$ has been defined on $L^2(\mathbb{R}^d)$ and $\hat{x}$ the generator of translation on it; or equivalently, one may regard $\hat{x}$ to be defined on $L^2(\Sigma_{(0)})$ and $\hat{p}$ the generator on it.) The dimensionality is given by $[\lambda^2]$. Note that this annihilation operator has nothing to do with the field annihilation operator in Eq. (2). We see that $[\hat{a}_i, \hat{a}_j^\dagger] = 2 |\lambda^2| \delta_{ij}$ and $[\hat{a}_i^\dagger, \hat{a}_j] = [\hat{a}_j^\dagger, \hat{a}_i] = 0$.

A coherent state is a normalizable physical state that is defined in $L^2(\mathbb{R}^d)$ or equivalently in $L^2(\Sigma_{(0)})$ by

$$
\hat{a} |\alpha\rangle = \alpha |\alpha\rangle,
$$

where $\alpha = (\alpha_1, \ldots, \alpha_d)$ is a $d$-vector of complex numbers of mass dimension $[\alpha] = [\lambda]$. From

$$
\lambda \left( \frac{x}{\sqrt{\sigma}} + \sqrt{\sigma} \nabla \right) \langle x | \alpha \rangle = \alpha \langle x | \alpha \rangle,
$$

we get the solution in $L^2(\Sigma_{(0)})$:

$$
\langle x | \alpha \rangle = \frac{1}{(\pi \sigma)^{\frac{d}{2}}} e^{-\frac{1}{2}(\frac{x}{\sqrt{\sigma}} - \beta)^2} e^{i\frac{\lambda}{\sqrt{\sigma}} \frac{x}{\sqrt{\sigma}}},
$$

where we have normalized such that $\langle \alpha | \alpha \rangle = 1$ and hence $[|\alpha\rangle] = 0$. In the momentum space $L^2(\mathbb{R}^d)$, this becomes

$$
\langle p | \alpha \rangle = \left( \frac{\sigma}{\pi} \right)^{\frac{d}{4}} e^{-i\sqrt{\sigma} p \cdot \beta} e^{-\frac{1}{2}((\sqrt{\sigma} p - \beta)^2)},
$$

de Eq. (55). Physically, the real and imaginary parts of $\alpha$ correspond to the center of position and momentum of the Gaussian wave packet. Looking at Eqs. (68) and (69), it is rather mysterious why the wave functions take such particular forms as functions of complex numbers $\alpha$. We will shed some light on this point in Sect. 3.

Comparing Eq. (68) with Eq. (58), we see that the Gaussian wave-packet state is indeed a coherent state in $L^2(\mathbb{R}^d)$.

14 The abuse of notation should be understood in that these $\alpha$, which are just numbers, have nothing to do with the Lorentz-friendly annihilation operator (25). Historically, the name “coherent state” comes from the one in field space that describes a photon coherent wave, rather than the one (66) in position–momentum space; see the paragraph containing Eq. (74).
or equivalently in $L^2(\Sigma(0))$:

$$|X, P\rangle = \left| \frac{X}{\sqrt{\sigma}} + i\sqrt{\alpha} P \right\rangle.$$  \hspace{1cm} (70)

By taking $\lambda = \sqrt{\sigma}$ and $-i/\sqrt{\sigma}$, we may write

$$|X, P\rangle = |X + i\sigma P\rangle_{\lambda=\sqrt{\sigma}} = \left| P - i \frac{X}{\sigma} \right\rangle_{\lambda=-i/\sqrt{\sigma}}.$$  \hspace{1cm} (71)

Now we see that the completeness relation (62) is equivalent to the completeness of the coherent states in $L^2(\mathbb{R}^d)$ or equivalently in $L^2(\Sigma(0))$:

$$\frac{1}{(2\pi |\lambda|^2)^d} \int d^d\alpha \left| \alpha \right\rangle \langle \alpha \right| = \mathbb{1},$$  \hspace{1cm} (72)

where

$$d^d\alpha = \prod_{i=1}^d d\alpha_i d\tilde{\alpha}_i = \sqrt{\prod_{i=1}^d \left(\frac{i}{2} d\alpha_i \wedge d\tilde{\alpha}_i\right)}.$$  \hspace{1cm} (73)

We list some more usable facts in Appendix A.  We comment that the coherent state in the position–momentum coherent state.

3 Lorentz-invariant wave packet

From the form of the Gaussian wave-packet state (56), it is tempting to generalize it into a Lorentz invariant form:

$$\langle p | X, P \rangle \propto e^{-i p \cdot X - \frac{1}{2} (p-P)^2} \to e^{-i p \cdot X - \frac{1}{2} (p-P)^2}$$

$$= e^{i \sigma^2} e^{-i p \cdot (X + i\sigma P)},$$  \hspace{1cm} (75)

where we have used the on-shell condition $p^2 = P^2 = -m^2$.  As we have seen in Eq. (71), the Gaussian wave-packet state $|X, P\rangle$ is nothing but a position–momentum coherent state.  For the coherent state, it is rather mysterious why the real and imaginary parts of the complex numbers $\alpha$ appear in the forms (68) and (69).  It is remarkable that the Lorentz invariant generalization (75) has the seemingly holomorphic dependence on the $D$ complex variables $X + i\sigma P$ if one generalizes $P$ to be off-shell.$^{15}$

Motivated by this fact, we define the following Lorentz-invariant wave-packet state in $L^2(\mathbb{R}^d)$:

$$\langle p | \sigma; X, P \rangle := N_\sigma e^{-i p \cdot (X + i\sigma P)}$$

$$= N_\sigma e^{i E_P X^0 - i p \cdot X} e^{-\sigma (E_P E_P - p^2)},$$  \hspace{1cm} (76)

where $N_\sigma$ is a normalization constant.  Given the reference frame $x$, this wave packet is centered near $x = X$ and $p = P$ at time $x^0 = X^0$.  As said above, one might want to regard the state $|\sigma; X, P\rangle$ as a basis of $\Sigma(\chi_0)$ in the interaction picture but we will see that, in terms of the wave function (104) in $\Sigma(\chi_0)$, $X^0$ is merely a parameter that specifies the wave packet $|\sigma; X, P\rangle$, while the time is specified by $x^0$.  Also, we will continue to abbreviate $\sigma$ to write $|X, P\rangle$ unless otherwise stated.

As an illustration of the more general computation spelled out in Appendix B, we will show in Sect. 3.1 that the normalization

$$\| |X, P\rangle \|^2 = 1,$$  \hspace{1cm} (77)

in $L^2(\mathbb{R}^d)$, is realized by

$$N_\sigma = \left(\frac{\sigma}{\pi}\right)^{\frac{d+1}{2}} \left(K_{\frac{d+1}{2}}(2\sigma m^2)\right)^{-\frac{1}{2}},$$  \hspace{1cm} (78)

where $K$ is the modified Bessel function of the second kind.  With this normalization, mass dimensions are $[|X, P\rangle] = 0$ and $[N_\sigma] = -\frac{d+1}{2}$.

We comment on possible generalizations of $P$ to be off-shell.  If we make $P$ off-shell in the first line in Eq. (76), it becomes divergent for $|p| \to \infty$ when $p \cdot P > 0$, namely, when

$$P^0 < v \cdot P,$$  \hspace{1cm} (79)

where $v := p/E_P$ with $|v| < 1$.  Therefore, the generalization of $P$ to off-shell would be safe so long as $P$ is timelike and future-oriented, in which case the condition (79) is never met.  (This is the case too if we let $P$ be off-shell in $e^{-i p \cdot X - \frac{1}{2} (p-P)^2} = e^{-i p \cdot X} e^{i \sigma^2 m^2 + \alpha p \cdot P}$, though the limit of super-heavy “off-shell mass” $P^2 \to \infty$ diverges.)

$^{15}$ As we will discuss below, the generalization of $P$ to an off-shell momentum is straightforward so far as $P$ is timelike and future-oriented.  We leave further generalization for future study.

$^{16}$ To be precise, the state $|\sigma; X, P\rangle$ is Lorentz covariant and the wave function (76) is Lorentz invariant.
3.1 Normalization

We compute the norm on $L^2(\mathbb{R}^d)$:

$$
\|X, P\|^2 = \int \frac{d^d p}{2E_p} \langle X, P | p \rangle \langle p | X, P \rangle 
= |N_{\sigma}|^2 \int \frac{d^d p}{2E_p} e^{2\sigma P \cdot p} 
= |N_{\sigma}|^2 \int d^D p \theta(p^0) \delta\left(p^2 + m^2\right) e^{2\sigma P \cdot p},
$$

(80)

where we let $p$ be off-shell in the last line to make the Lorentz invariance manifest. As $P$ is on-shell, we may always find a Lorentz transformation $\Lambda(P)$ to its rest frame $\tilde{P} := (m, 0)$ such that $\Lambda P = \tilde{P}$. Then we change the integration variable to $\tilde{P} := \tilde{P} - \pi z$.

Let us compute the inner product of two Lorentz invariant wave packets $(76)$ comes back to the Gaussian form $(56)$ up to the factor $\sqrt{2m}$,

$$
\langle p | X, P \rangle \rightarrow \sqrt{2m} \left(\frac{\sigma}{\pi}\right)^{\frac{d-1}{2}} e^{\frac{1}{4} \frac{m}{\sqrt{\sigma}} e^{-ipX_0 - ipX - \frac{1}{2} (p - \tilde{P})^2}},
$$

(84)

where $E_p = m + \frac{p^2}{2m} + \cdots$, we have used the limit (83), and have neglected $O(m^{-2})$ terms in the last exponent in Eq. (84). In the ultra-relativistic limit, $m \rightarrow 0$, we get

$$
\langle p | X, P \rangle \rightarrow \sqrt{2m} \left(\frac{\sigma}{\pi}\right)^{\frac{d-1}{2}} e^{-|p||p||1 - \cos \theta_P - iX_0 - X_0| \cos \theta_X},
$$

(85)

where $\cos \theta_X := p \cdot X / |p||X|$ and $\cos \theta_P := p \cdot P / |p||P|$. In this limit, the original Gaussian suppression is made weaker. Especially along the direction of $P$, $\cos \theta_P = 1$, there is no suppression for a large momentum $|p| \rightarrow \infty$.

This is the main obstacle of having a Lorentz-invariant wave packet for a massless particle.

3.2 Inner product

Let us compute the inner product of two Lorentz invariant wave packets: $\langle \sigma ; X, P | \sigma' ; X', P' \rangle$ on $L^2(\mathbb{R}^d)$. Here and hereafter, a prime symbol $'$ never denotes a derivative.

Motivated by the coherent states in the position–momentum space $(71)$, we define the following complex variables:

$$
Z^\mu(\sigma) := X^\mu + i\sigma P^\mu, \quad \Pi^\mu(\sigma) := P^\mu - i \frac{X^\mu}{\sigma},
$$

(86)

(87)

which are related by $Z^\mu = i\sigma \Pi^\mu$. We define the Lorentz invariant analog of the coherent state $(71)$: \(^17\)

$$
|Z(\sigma)\rangle := |\sigma ; X, P\rangle, \quad |\Pi(\sigma)\rangle := |\sigma ; X, P\rangle.
$$

(88)

We see that

$$
\langle p | Z(\sigma) \rangle = N_{\sigma} e^{-ipZ(\sigma)}, \quad \langle p | \Pi(\sigma) \rangle = N_{\sigma} e^{ip\Pi(\sigma)}.
$$

(89)

For later use, we define the “norm” of an arbitrary complex $D$-vector $\Xi$:

$$
\|\Xi\| := \sqrt{-\Xi^2} = \sqrt{(\xi^0)^2 - \Xi^2},
$$

(90)

\(^17\) Abuse of notation is understood: always the first and second definitions in Eq. (88) are used for the arguments $Z$ and $\Pi$, respectively.
which is not necessarily positive nor even a real number.\footnote{The abuse of notation should be understood: This has nothing to do with the norm of a state vector in the Hilbert space such as in Eq. (77).} Now we may write

$$\{ \sigma; X, P \mid \sigma'; X', P' \} = \{ \Pi(\sigma) \mid \Pi'(\sigma') \} = N_{\sigma} N_{\sigma'} \int \frac{d^2p}{2E_p} e^{iP \cdot (\sigma \Pi(\sigma) + \sigma' \Pi'(\sigma'))}.$$  \hfill(91)

To compute this, it is convenient to define the master integral:

$$\mathcal{I}(\Xi) := \int \frac{d^2u}{2u^0} e^{i u \cdot \Xi} = \int d^D u \, \delta(u^2 + 1) \, \theta(u^0) \, e^{i u \cdot \Xi},$$  \hfill(92)

where $\Xi$ is a dimensionless complex $D$-vector and the $D$-vector $u (= p/m)$ is on-shell and off-shell for the first and second integrals, respectively. In Appendix B, we present a detailed evaluation of the integral, and the result is

$$\mathcal{I}(\Xi) = (2\pi)^{D/2} \frac{K_{D/2}(\|\Xi\|)}{\|\Xi\|^{D/2}},$$  \hfill(93)

which is valid when $\Re \Xi$ is timelike ($\Re\Xi^2 < 0$) and future-oriented $\Im \Xi^0 > 0$. This also implies that

$$\mathcal{I}(2\sigma m) = \frac{1}{m^{D-1} N_{\sigma}}.$$  \hfill(94)

with $N_{\sigma}$ is given in Eq. (78).

The integral in the inner product (91) corresponds to

$$\Xi = m \left( \sigma \Pi^*(\sigma) + \sigma' \Pi'(\sigma') \right) = i m \left( Z^*(\sigma) - Z'(\sigma') \right),$$  \hfill(95)

that is,

$$\Re \Xi = m \left( \sigma P + \sigma' P' \right), \quad \Im \Xi = m \left( X - X' \right).$$  \hfill(96)

From

$$\begin{align*}
(\sigma P + \sigma' P')^2 &= -\left( \sigma^2 + \sigma'^2 \right) m^2 + 2\sigma \sigma' P \cdot P' \\
&\leq -\left( \sigma^2 + \sigma'^2 \right) m^2 + 2\sigma \sigma' \\
&\times \left( -\sqrt{|P|^2 + m^2} \sqrt{|P'|^2 + m^2} + |P| |P'| \right) < 0,
\end{align*}$$  \hfill(97)

we see that $\Re \Xi$ is always timelike. Therefore we may use the result (93):

$$\{ \sigma; X, P \mid \sigma'; X', P' \} = N_{\sigma} N_{\sigma'} (2\pi)^{D/2} m^{D-1} \frac{K_{D/2}(\|\Xi\|)}{\|\Xi\|^{D/2}},$$  \hfill(98)

where, in various notations,

$$\|\Xi\|^2 = -\Xi^2 = -m^2 \left( \sigma \Pi^* + \sigma' \Pi' \right)^2$$

$$= m^2 (Z^* - Z')^2$$

$$= -m^2 (\sigma P + \sigma' P' + i (X - X')^2$$

$$= m^2 ((X - X') - i(\sigma P + \sigma' P')^2.)$$  \hfill(99)

Especially when $\sigma = \sigma'$, we have

$$\{ X, P \mid X', P' \} = \frac{(2\sigma m^2)^{D/2} K_{D/2}(\|\Xi\|)}{K_{D/2}(2\sigma m^2)} \frac{\|\Xi\|^{D/2}}{\|\Xi\|^{D/2}},$$  \hfill(100)

where

$$\|\Xi\|^2 = -m^2 \sigma^2 (\Pi^* + \Pi')^2$$

$$= m^2 (Z^* - Z')^2$$

$$= -m^2 (\sigma (P + P') + i (X - X')^2$$

$$= m^2 ((X - X') - i(\sigma (P + P'))^2.$$

3.3 Wave function

Let us compute the wave function for the Lorentz-invariant wave-packet state on $L^2(\Sigma_{\mu,\nu})$:

$$\langle x \mid X, P \rangle = \int \frac{d^D p}{2E_p} \langle x \mid p \rangle \langle p \mid X, P \rangle$$

$$= \frac{N_{\sigma}}{(2\pi)^D} \int \frac{d^D p}{2E_p} e^{i P + i(x-X)}.$$  \hfill(102)

Comparing with Eq. (92), we see the following correspondence:

$$\Xi = m(\sigma P + i(x - X)).$$  \hfill(103)

Obviously $(\Re \Xi)^2 = -\sigma^2 m^4 < 0$, and we may use Eq. (93):

$$\langle x \mid X, P \rangle = \frac{N_{\sigma} m^{D/2} K_{D/2}(\|\Xi\|)}{\sqrt{2\pi}} \|\Xi\|^{D/2}.$$  \hfill(104)
we get
\[ \parallel \Xi \parallel = \sqrt{-\mathcal{E}^2} = m \sqrt{\sigma^2 m^2 + (x - X)^2 - 2i \sigma P \cdot (x - X)}. \]

The explicit form of the wave function (104) is one of our main results. This reduces to the earlier one in Refs. [16,17] when \( d = 3 \) in the \( X \to 0 \) limit and may be interpreted as its spacetime translation by \( X \). We note that there is no branch-cut ambiguity for the argument (105) as long as \( m > 0 \); see the last paragraph in Appendix B.1.

Hereafter, we examine various characteristics of the above wave function. Firstly, along the line \( x = X + Ps \) corresponding to the particle trajectory, with \( s \) being a real parameter, we get \( \Xi = mP (\sigma + is) \) and hence \( \parallel \Xi \parallel = m^2 (\sigma + is) \). For a point sufficiently apart from \( X \) along this trajectory, namely for \( s \to \pm \infty \), we get
\[ \langle x | X, P \rangle \sim \frac{(\frac{\sigma}{\pi})^{\frac{d-1}{2}}}{2m \sqrt{K_{\frac{d-1}{2}}(2\sigma m^2)}} e^{-m^2(\sigma + is)} \cdot \exp \left[ -\frac{\sigma}{2(s^2 + \sigma^2)} \left( e^2 + \left( \frac{L}{m} \cdot \epsilon \right)^2 \right) \right]. \]

It is noteworthy that the more we go along the trajectory \( x = X + s P \) (namely the larger the \( |s| \) is), the larger the spatial width-squared \( \sim (s^2 + \sigma^2) / \sigma \) of this Gaussian factor becomes.

For a wave-packet scattering, we may parametrize each of the incoming waves, \( a \), and of the outgoing ones, \( b \), such that the scattering occurs (i.e. the wave packets overlap) around finite region \( |s_a| \sim |s_b| < \infty \). If the scattering occurs within a large time interval, the in and out asymptotic states are given by \( s_a \to -\infty \) and \( s_b \to \infty \), respectively. In such a case, we may approximate an in-coming/out-going wave packet by the near plane wave (107) better and better, whereas they still interact as wave packets rather than plane waves.

Thirdly, for the plane-wave expansion with large \( \sigma \), the argument becomes
\[ \langle x | X, P \rangle \sim \frac{(\frac{\sigma}{\pi})^{\frac{d}{2}}}{\sqrt{2} (\sigma m)^{d-\frac{1}{2}}} e^{iP \cdot (x - X) - \frac{1}{2} (x - X)^2 - \frac{(P \cdot (x - X))^2}{2m^2}. \]

The corresponding probability density is
\[ \langle | x \rangle | \sqrt{2} \hat{E}_{\hat{P}} | X, P \rangle \sim \frac{E P (\frac{\sigma}{\pi})^d}{(\sigma m)^{d-\frac{1}{2}}} e^{-\frac{1}{2} (x - X)^2 - \frac{(P \cdot (x - X))^2}{2m^2}}, \]

where we have used the completeness (37).

In particular on the line \( x = X + Ps \), with \( s \) being a real parameter, the quadratic terms of \( s \) cancel out in the exponent in Eq. (109):
\[ \langle x | X, P \rangle \sim \frac{(\frac{\sigma}{\pi})^d}{\sqrt{2} (\sigma m)^{d-\frac{1}{2}}} e^{-im^2s}. \]

As promised, we have confirmed that the wave function does not receive the Gaussian suppression along this particle trajectory. We stress that in this sense, the Lorentz-invariant wave packet is not localized in time, just as the Gaussian wave packet reviewed in Sect. 2.3.

19 On the other hand, when we take the non-relativistic limit \( m \to \infty \) first, we get \( \parallel \Xi \parallel = \sigma m^2 + im (x^0 - X^0) - i P \cdot (x - X) + \frac{i m X}{2m^2} + O(\frac{1}{\sigma}). \)
If we furthermore take the non-relativistic limit in the exponent of the large-σ expansion (109), it becomes

\[ i P \cdot (x - X) - \frac{(x - X - V(x^0 - X^0))^2}{2\sigma} - \frac{(V \cdot (x - X))^2}{2\sigma} + O(|V|^3), \quad (112) \]

where \( P^0 = m + \frac{m}{2} V^2 + \cdots \). Comparing with the Gaussian wave packet (60), we see that the extra suppression factor

\[ \exp \left( -\frac{(V \cdot (x - X))^2}{2\sigma} \right) \quad (113) \]

appears from the Lorentz-invariant wave packet, and the center of the Lorentz-invariant wave packet departs from the particle trajectory \( X - V(x^0 - X^0) \) of the Gaussian wave packet (60).

Finally, in the particle/ultra-relativistic limit \( \sigma m^2 \to 0 \), we get

\[ \langle x \mid X, P \rangle \to \frac{(\sigma m^2)^{\frac{d-1}{2}} K_{d-1}(\|\Xi\|)}{\sqrt{(d-1)!} \|\Xi\|^\frac{d-1}{2}}, \quad (114) \]

where the argument goes to \( \|\Xi\| \to m \sqrt{(x - X)^2 - 2i\sigma P \cdot (x - X)} \). If we furthermore take the relativistic limit \( m \to 0 \), we get.\(^{20}\) We have

\[ \langle x \mid X, P \rangle \to \frac{\sqrt{(x - X)^2 - 2i\sigma P \cdot (x - X)}}{(1 - i \frac{\sigma P \cdot (x - X)}{(x - X)^2}) \mp \cdots}; \]

when timelike, \( (x - X)^2 < 0 \),

\[ \|\Xi\| \to -im \text{ sgn}(P \cdot (x - X)) \sqrt{-(x - X)^2} \left( 1 + i \frac{\sigma P \cdot (x - X)}{(x - X)^2} + \cdots \right); \]

and when lightlike \( (x - X)^2 = 0 \),

\[ \|\Xi\| \to m \sqrt{2i\sigma P \cdot (x - X)} \left( 1 + i \frac{\sigma m^2}{4P \cdot (x - X)} + \cdots \right). \]

\(^{20}\) On the other hand, first taking the particle limit \( \sigma \to 0 \) is tricky due to the branch cut: When \( x \) is located at a spacelike distance from \( X \), namely \( (x - X)^2 > 0 \),

\[ \|\Xi\| \to m \sqrt{(x - X)^2} \left( 1 - i \frac{\sigma P \cdot (x - X)}{(x - X)^2} + \cdots \right); \]

As we only consider free propagation of the waves, \( \hat{H} = \hat{H}_{\text{free}} \), this is the same as

\[ \langle \hat{O}_I(x^0) \rangle := \langle X, P \mid e^{i\hat{H}_{\text{free}} x^0} \hat{O} e^{-i\hat{H}_{\text{free}} x^0} \mid X, P \rangle. \quad (118) \]

for our application. In particular when \( \hat{O} \) only contains momentum operators such that \( \left[ \hat{O}, \hat{H}_{\text{free}} \right] = 0 \), the expectation value becomes time independent, \( \langle \hat{O} \rangle = \langle \hat{O}_I(x^0) \rangle \).

First, we write

\[ \langle \hat{p}^{\mu_1} \cdots \hat{p}^{\mu_n} \rangle = \int \frac{d^d p}{2E_p} \langle \langle p \mid X, P \rangle \mid^2 p^{\mu_1} \cdots p^{\mu_n} \]

\[ = N^2 \sigma^{d-1+n} \int \frac{d^d u}{2u^0} e^{2\sigma m P \cdot u} u^{\mu_1} \cdots u^{\mu_n}, \quad (120) \]
where $u = p/m$ is the $D$-velocity with $u^0 = \sqrt{1 + u^2}$. To compute the above, we take derivatives of the master integral (93):

$$T_{\mu_1 \cdots \mu_n}(\Xi) := \frac{\partial^n}{\partial \Xi_{\mu_1} \cdots \partial \Xi_{\mu_n}} T(\Xi) = \int \frac{d^d u}{(2\pi)^d} e^{i u \cdot \Xi} u_{\mu_1} \cdots u_{\mu_n},$$

(121)

where $\Xi$ is off-shell. Once this is obtained, we may substitute $\Xi = 2\sigma m P$, which is “on-shell”, $\| \Xi \| = \sqrt{-\Xi^2} = 2\sigma m^2$.

From Eqs. (205) and (206) in Appendix B, we read

$$\langle \hat{P}_\mu \rangle = \frac{T^\mu(2\sigma m P)}{T(2\sigma m P)}$$

(122)

and hence,

$$\langle \hat{P}_\mu \hat{P}_\nu \rangle - \langle \hat{P}_\mu \rangle \langle \hat{P}_\nu \rangle = \frac{\eta_{\mu \nu} K_{d+1}(\| \Xi \|)}{2\sigma K_{d-1}(\| \Xi \|)} + \frac{P^\mu P^\nu}{K_{d+1}(\| \Xi \|) K_{d-1}(\| \Xi \|)} \left( \frac{K_{d+1}(\| \Xi \|)}{K_{d-1}(\| \Xi \|)} \right)^2.$$

(123)

Note that contraction of Eq. (123) with the flat metric $\eta_{\mu \nu}$ gives $\eta_{\mu \nu} \langle \hat{P}_\mu \hat{P}_\nu \rangle = -m^2$ as it should, due to the Bessel identity (208). We see that, for a fixed $\sigma$ and $m$, the (co)variance (124) becomes larger and larger for $|P| \to \infty$ due to the second term. Furthermore, even the off-diagonal covariance for $\mu \neq \nu$ is non-zero. This is due to the fact that, with $P \neq 0$, the Lorentz-invariant wave packet is boosted and is not spherically symmetric in the momentum space, unlike the Gaussian wave packet (56). The above results agree with Eqs. (4.4) and (4.5) in Ref. [6].

From Eq. (122), we obtain

$$\langle \hat{P}_\mu \rangle = \frac{\eta_{\mu \nu} K_{d+1}(\| \Xi \|)}{2\sigma K_{d-1}(\| \Xi \|)} + \frac{P^\mu}{K_{d+1}(\| \Xi \|) K_{d-1}(\| \Xi \|)} \left( \frac{K_{d+1}(\| \Xi \|)}{K_{d-1}(\| \Xi \|)} \right)^2.$$

(124)

where the equality holds in the plane-wave/non-relativistic limit $\| \Xi \| = 2\sigma m^2 \to \infty$. It is curious that the mass constructed from the expectation value of $D$-momentum $(\hat{P}_\mu)$ becomes larger than the “intrinsic” mass $m$, no matter whether the particle is at rest $P = 0$ or not. This fact has been pointed out in Ref. [17].

In the plane-wave/non-relativistic expansion for large $\| \Xi \| = 2\sigma m^2$, we get

$$\langle \hat{P}_\mu \rangle = \left( 1 + \frac{d}{2 \| \Xi \|} + \frac{d (d-2)}{8 \| \Xi \|^2} + \cdots \right) P^\mu,$$

(126)

and hence,

$$\langle \hat{P}_\mu \hat{P}_\nu \rangle = \frac{\eta_{\mu \nu}}{2\sigma} \left( 1 + \frac{d}{2 \| \Xi \|} + \frac{d (d-2)}{8 \| \Xi \|^2} + \cdots \right) + \frac{P^\mu P^\nu}{\| \Xi \|} \left( \frac{1}{\| \Xi \|^2} + \frac{d (d+1)}{2 \| \Xi \|^3} + \cdots \right),$$

(127)

where the dots denote terms of order $\| \Xi \|^{-3}$. As a cross-check, we can derive from Eq. (127) that

$$\langle \hat{P}^2 + m^2 \rangle = \frac{d}{2\sigma} + P^2 + m^2 + \frac{d+1}{2\sigma m^2} P^2 + O\left( \frac{1}{\sigma^2} \right),$$

(129)

and we see that the two coincide.

We show the result of the plane-wave expansion with large $\sigma$ in Eq. (124):

$$\langle \hat{P}_\mu \hat{P}_\nu \rangle = \frac{1}{2\sigma} \left( \eta_{\mu \nu} + \frac{P^\mu P^\nu}{m^2} \right) + \frac{d}{8\sigma^2 m^2} \left( \eta_{\mu \nu} + \frac{2P^\mu P^\nu}{m^2} \right) + O\left( \frac{1}{\sigma^3} \right).$$

(131)

That is,

$$\langle \hat{P}_i \hat{P}_j \rangle - \langle \hat{P}_i \rangle \langle \hat{P}_j \rangle = \frac{1}{2\sigma} \left( \delta_{ij} + \frac{P_i P_j}{m^2} \right) + \frac{d}{8\sigma^2 m^2} \left( 1 + \frac{2P_i P_j}{m^2} \right) + O\left( \frac{1}{\sigma^3} \right),$$

(132)

where

$$\langle \hat{P}^0 \rangle^2 - \langle \hat{P}_i \rangle \langle \hat{P}_i \rangle = \frac{P^2}{2\sigma m^2}.$$
Now let us compute the expectation value
\[ E \uparrow \text{ Gaussian wave packet, which is spherically symmetric } \propto \delta_{ij}. \]
The second term shows that even the off-diagonal covariance for \( i \neq j \) is non-zero, due to the boost in the momentum space mentioned above. The first term in the energy variance (133) is also due to the boost, and it is canceled out when we take the Lorentz invariant combination \( \mathcal{p}^2 - \mathcal{p}^2 \): By subtracting the two sides of Eq. (133) from those of Eq. (134) contracted with \( \delta_{ij} \), we obtain
\[
- \mathcal{p}^2 = m^2 + \frac{d}{2\alpha} + \frac{d(d-1)}{8\sigma^2 m^2} + \cdots .
\]
(136)

As mentioned above, we see that the mass constructed from the expectation value of \( \mathcal{p}^2 \) is increased from the intrinsic mass \( m \).

### 4.2 Position (co)variance

Now let us compute the expectation value \( \langle \hat{x}^i \rangle \) and its covariance:
\[
\langle \langle \hat{x}^i - \langle \hat{x}^i \rangle \rangle \langle \hat{x}^j - \langle \hat{x}^j \rangle \rangle \rangle = \langle \hat{x}^i \rangle \langle \hat{x}^j \rangle - \langle \hat{x}^i \rangle \langle \hat{x}^j \rangle .
\]
(137)

First,
\[
\langle \hat{x}_i \rangle = \int \frac{d^d p}{2E_p} \langle \langle X, P | p \rangle \langle p | \hat{x}_i | X, P \rangle \rangle
\]
\[
= \int \frac{d^d p}{2E_p} \langle \langle X, P | p \rangle \langle p | \hat{x}_i | X, P \rangle \rangle i \left( \frac{\partial}{\partial p_i} - \frac{p_i}{2E_p} \right) \langle p | X, P \rangle
\]
\[
= X_i - \left( \frac{u^i}{u^0} \right) X^0 ,
\]
(138)

where we write
\[
\left( \frac{u^i}{u^0} \right)^n := m^{n-1} \left( \frac{\mathcal{p}^i}{\mathcal{p}^0} \right)^n .
\]
(139)

and we have used the following identity:21
\[
2m\sigma P^i - 2m\sigma E_p \left( \frac{u^i}{u^0} \right) - \left( \frac{u^i}{u^0} \right) = 0 .
\]
(140)

We have defined \( \hat{x} \) as a time-independent Schrödinger-picture operator in a certain frame. Therefore the expectation value (138) should correspond to measurement in an equal-time slice in this frame, and hence the appearance of the non-covariant velocity \( \left( \frac{\mathcal{u}^i}{\mathcal{u}^0} \right) \) rather than the covariant one \( \left( \frac{u^i}{u^0} \right) \). As we identify the Schrödinger, Heisenberg, and interaction pictures at \( x^0 = 0 \), the expectation value (138) corresponds to the measurement on the spacelike hyperplane \( \Sigma(0) \). If we instead consider the time-dependent operator \( \hat{x}_1(x^0) := e^{i\hat{H}_\text{heat} x^0} \hat{x} e^{-i\hat{H}_\text{heat} x^0} \) in the interaction picture, we obtain
\[
\langle \langle \hat{x}_1(x^0) \rangle \rangle = \int \frac{d^d p}{2E_p} \langle \langle X, P | p \rangle \langle p | e^{i\hat{H}_\text{heat} x^0} \hat{x} e^{-i\hat{H}_\text{heat} x^0} | X, P \rangle \rangle
\]
\[
= X_i + \left( \frac{u^i}{u^0} \right) (x^0 - X^0) .
\]
(141)

Second, we may similarly compute
\[
\langle \langle \hat{x}_i \rangle \rangle = \int \frac{d^d p}{2E_p} \left( \frac{\partial}{\partial p^i} \langle \langle X, P | p \rangle \langle p | X, P \rangle \rangle \right) \left( \frac{\partial}{\partial p^j} \langle \langle X, P | p \rangle \langle p | X, P \rangle \rangle \right)
\]
\[
= N^2 m^{d-3} \int d^d u \left( \frac{\partial}{\partial u^i} e^{iu \cdot (\sigma P - X)} \right) \left( \frac{\partial}{\partial u^j} e^{iu \cdot (\sigma P - X)} \right)
\]
\[
\times \left( \frac{\partial}{\partial u^0} e^{iu \cdot X} \right) .
\]
(142)

Using \( \frac{\partial}{\partial u^i} e^{iu \cdot (\sigma P - X)} = e^{iu \cdot P} \left( \frac{\partial}{\partial u^i} e^{iu \cdot X} \right) + im \left( \frac{\partial}{\partial u^i} e^{iu \cdot P} / \partial u^0 \right) \), we can show that \( \langle \langle \hat{x}_i \rangle \rangle = 0 \). Then we obtain
\[
\langle \langle \hat{x}_i \rangle \rangle = \left( \langle \langle \left( \sigma P_i - P^0 u_i / u^0 - \frac{u_i}{u^0} \right) - \frac{u_j}{u^0} \right) \left( \langle \langle X_j - X^0 u_j / u^0 - \frac{u_j}{u^0} \rangle \rangle \right) \right)
\]
\[
= \left( \sigma P_i - P^0 u_i / u^0 - \frac{u_i}{u^0} \right) \left( X_j - X^0 u_j / u^0 - \frac{u_j}{u^0} \right) .
\]

21 This may be derived for a general (timelike) D-vector \( \Sigma \) as
\[
\int \frac{d^d u}{2d^d u} e^{u \cdot \Sigma} \left( \begin{array}{c} \Sigma - \Sigma^0 \frac{u^i}{u^0} \end{array} \right) = \int \frac{d^d u}{2u^0} \left( \frac{\partial}{\partial u^i} \right) \left( \begin{array}{c} \Sigma^0 \frac{u^i}{u^0} \end{array} \right) = 0 .
\]
(143)

and then putting the “on-shell” value \( \Sigma = 2\sigma m P \). Recall that \( P \) and \( u \) are on-shell.
\[= X_i X_j + \left( X_0 \right)^2 \left( \frac{u_i u_j}{\langle u^2 \rangle} \right) - X_i X_0 \left( \frac{u_i}{\langle u^2 \rangle} \right) - X_j X_0 \left( \frac{u_j}{\langle u^2 \rangle} \right) + \sigma^2 P_i P_j - \sigma^2 \left( \frac{u_i}{\langle u^2 \rangle} \right) P^0 P_j - \sigma^2 \left( \frac{u_j}{\langle u^2 \rangle} \right) P^0 P_i + \sigma^2 \left( P^0 \right)^2 \left( \frac{u_i u_j}{\langle u^2 \rangle^2} \right) - \frac{\sigma P_i}{2 m} \left( \frac{u_i}{\langle u^2 \rangle} \right) - \frac{\sigma P_j}{2 m} \left( \frac{u_j}{\langle u^2 \rangle} \right) + \frac{\sigma P^0}{m} \left( \frac{u_i u_j}{\langle u^2 \rangle^3} \right) + \frac{1}{4 m^2} \frac{u_i u_j}{\langle u^2 \rangle^4}, \tag{143} \]

and hence\textsuperscript{22}

\[
\left\langle \hat{x}^i \hat{x}^j \right\rangle - \left\langle \hat{x}^i \right\rangle \left\langle \hat{x}^j \right\rangle = \left( X_0 \right)^2 \left( \left( \frac{u_i u_j}{\langle u^2 \rangle^2} \right) - \left( \frac{u_i}{\langle u^2 \rangle} \right) \left( \frac{u_j}{\langle u^2 \rangle} \right) \right) - \sigma^2 P_i P_j + \sigma^2 \left( P^0 \right)^2 \left( \frac{u_i u_j}{\langle u^2 \rangle^2} \right) + \frac{\sigma P^0}{m} \left( \frac{u_i u_j}{\langle u^2 \rangle^3} \right) + \frac{1}{4 m^2} \frac{u_i u_j}{\langle u^2 \rangle^4}, \tag{144} \]

where we have used the identities (140) and

\[0 = 2 m \sigma P_i \left( \frac{1}{\langle u^2 \rangle^{n-1}} \right) - 2 m \sigma P^0 \left( \frac{u_i}{\langle u^2 \rangle^{n+1}} \right) - n \left( \frac{u_i}{\langle u^2 \rangle^{n+1}} \right), \tag{145} \]

In this paper, we compute the expectation value (138) and the (co)variance (144) using the saddle-point method for large \( \sigma \):

\[
\left\langle \hat{x}^i \right\rangle = X^i - X_0 \frac{P^i}{P^0} \left[ 1 - \frac{1}{2 \sigma} \frac{1}{(P^0)^2} + \mathcal{O} \left( \frac{1}{\sigma^2} \right) \right], \tag{146} \]

\[
\left\langle \hat{x}^i \hat{x}^j \right\rangle - \left\langle \hat{x}^i \right\rangle \left\langle \hat{x}^j \right\rangle = \frac{\sigma}{2} \left( \delta_{ij} - \frac{P_i P_j}{(P^0)^2} \right) + \mathcal{O} \left( \sigma^0 \right). \tag{147} \]

Especially for the variance \( i = j \),

\[
\left\langle \hat{x}^i \right\rangle^2 - \left\langle \hat{x}^i \right\rangle^2 = \frac{\sigma}{2} \left( 1 - \frac{P^2}{P^0} \right) + \mathcal{O} \left( \sigma^0 \right), \tag{148} \]

where \( i \) is not summed. One may find the detailed derivation in Appendix B. Especially, we have used Eq. (255) to compute \( \left( \frac{u_i}{\langle u^2 \rangle} \right) = \frac{T_i}{T_0} = \frac{g_i}{E^0} \left( 1 - \frac{1}{m^2} \langle \xi^2 \rangle + \cdots \right) \) with \( \Xi = 2 m \sigma P \) and \( \| \Xi \| = 2 \sigma m^2 \) for \( \langle \hat{x}^i \rangle \), and similarly Eq. (256) for \( \langle \hat{x}^i \hat{x}^j \rangle \). The result (148) implies that if we measure the position uncertainty along the direction of \( \boldsymbol{P} \), it is Lorentz-contracted by the factor \( m / E_P \), compared to the measurement transverse to \( \boldsymbol{P} \) [16, 17, 26].

4.3 Uncertainty relation

Finally combining Eqs. (132) and (148), the uncertainty relation on the time slice \( \Sigma_{(0)} \) becomes

\[
\sqrt{\left( \langle \hat{\xi}_i \rangle^2 \right) - \left\langle \hat{\xi}_i \right\rangle^2} \sqrt{\left( \langle \hat{\pi}_j \rangle^2 \right) - \left\langle \hat{\pi}_j \right\rangle^2} = \frac{1}{2} \sqrt{\left( 1 - \frac{P_i^2}{E^2_P} \right) \left( 1 + \frac{P_j^2}{m^2} \right) + \mathcal{O} \left( \frac{1}{\sigma} \right)}, \tag{149} \]

where \( i \) is not summed. In the non-relativistic limit, we see that the terms of order \( P^2 / m^2 \) cancel out:

\[
\sqrt{\left( \langle \hat{\xi}_i \rangle^2 \right) - \left\langle \hat{\xi}_i \right\rangle^2} \sqrt{\left( \langle \hat{\pi}_j \rangle^2 \right) - \left\langle \hat{\pi}_j \right\rangle^2} = \frac{1}{2} + \mathcal{O} \left( \frac{P^2}{m^4} \right), \tag{150} \]

where \( i \) is not summed. The ordinary minimum uncertainty for the Gaussian wave is recovered in the non-relativistic limit.

When we measure along a direction \( \boldsymbol{n} \) with \( |\boldsymbol{n}| = 1 \) and \( \boldsymbol{n} \cdot \boldsymbol{P} = |\boldsymbol{P}| \cos \theta \),

\[
\sqrt{\left( \langle \hat{\xi}_n \rangle^2 \right) - \left\langle \hat{\xi}_n \right\rangle^2} \sqrt{\left( \langle \hat{\pi}_n \rangle^2 \right) - \left\langle \hat{\pi}_n \right\rangle^2} = \frac{1}{2} \sqrt{\left( 1 - |\boldsymbol{P}|^2 \cos^2 \theta \right) \left( 1 + \frac{|\boldsymbol{P}|^2 \cos^2 \theta}{m^2} \right) + \mathcal{O} \left( \frac{1}{\sigma} \right)}, \tag{151} \]

where we write \( A_n := \boldsymbol{n} \cdot \boldsymbol{A} \) for any spatial vector \( \boldsymbol{A} \). We see that the uncertainty is minimized to \( 1 / 2 \) when we measure along the directions \( \theta = 0, \pi / 2, \) and \( \pi \); namely, when it is either parallel or perpendicular to \( \boldsymbol{P} \).

4.4 Time–energy uncertainty

Before proceeding, we comment on the time uncertainty. The Lorentz-invariant wave packet is not localized in time as discussed above, and therefore the expectation value of time \( \langle \hat{\xi}^0 \rangle \) for this wave packet is ill-defined, just as the expectation

\[
\frac{1}{4 m^2} \left( \frac{u_i u_j + 2 \langle u^2 \rangle \xi^0 \xi^i \xi^j}{\langle u^2 \rangle^2} \right) \]
value of position is ill-defined for a plane wave.\textsuperscript{23} However, we can show that the energy uncertainty (133) is matched with the uncertainty of the time at which this wave packet passes through a certain point \( x \). Suppose we are at \( x = X \) and see the wave packet passing through it around the time \( t^0 \sim X^0 \). Then the probability density on each \( \Sigma_{(t^0)} \) along the worldline \( x = X \) becomes

\[
\left| \langle x | \sqrt{2E_P} | X, P \rangle \right|^2 \approx \frac{(\pi \sigma_E)^{2d-1}}{(2\pi m)^{d-1}} e^{-\frac{1}{2}E_P \sigma^2 (t^0 - X^0)^2}. \tag{152}
\]

From the exponent, we see that the timelike width-squared is \((\Delta t)^2 \approx \frac{\sigma m^2}{\Delta \sigma^2} \). Comparing with the energy uncertainty (133), we see that the time–energy uncertainty takes the minimum value for the position–momentum one at the leading order:

\[
(\Delta t)^2 \Delta \sigma^2 \approx \frac{1}{2}. \tag{153}
\]

It would also be interesting to consider a wave-packet scattering. Then what is localized in time is not each wave packet but an overlap of the wave packets: This kind of time-like width-squared of the overlap region is given as \( \sigma_t \) in Ref. \cite{27} and as \( \sigma_\text{in}, \sigma_\text{out} \) in Refs. \cite{2,5} for the Gaussian wave packets. This will be pursued in a separate publication.

## 5 Completeness of Lorentz-invariant basis

Let us discuss the completeness on \( L^2(\mathbb{R}^d) \). We will prove the following manifestly Lorentz-invariant completeness relation:

\[
\int_{\Sigma_X} \frac{d^d \Sigma^\mu}{(2\pi)^d} \int \frac{d^d P}{2E_P} \langle p | X, P \rangle \left( 2i \frac{\partial}{\partial X^\mu} \right) \langle X, P | q \rangle = \langle p | q \rangle, \tag{154}
\]

where \( \Sigma_X \) is an arbitrary spacelike hyperplane in the \( X \) space and \( d^d \Sigma^\mu \) is a \( d \)-volume element that is normal to \( \Sigma_X \). In the language of differential forms, \( d^d \Sigma^\mu = - \star dX^\mu = -\frac{1}{d!} \epsilon_{\mu_1 \ldots \mu_d} dX^{\mu_1} \wedge \ldots \wedge dX^{\mu_d} \); see Eq. (38) and below; see also Ref. \cite{27} for discussion on Lorentz invariance of the phase space volume. In other words,

\[
\int_{\Sigma_X} \frac{d^d \Sigma^\mu}{(2\pi)^d} \int \frac{d^d P}{2E_P} \langle X, P \rangle \left( 2i \frac{\partial}{\partial X^\mu} \right) \langle X, P | \hat{1} \rangle = \hat{1}, \tag{155}
\]

where the right-hand side is the identity operator in the free one-particle subspace. Now the Lorentz-friendly plane wave is expanded as

\[
| p \rangle = \int \frac{d^d \Sigma^\mu}{(2\pi)^d} \int \frac{d^d P}{2E_P} | X, P \rangle \left( 2i \frac{\partial}{\partial X^\mu} \right) \langle X, P | p \rangle. \tag{156}
\]

The completeness (154) can be rewritten as

\[
N^2 \int_{\Sigma_X} \frac{-2q_\mu \Sigma^\mu}{(2\pi)^d} \int \frac{d^d P}{2E_P} e^{-i(p-q)X^0} e^{i\sigma(P+q)} e^{-i(p-q)X} e^{i\sigma(P+q)} = 2E_p \delta^d(p-q). \tag{157}
\]

The proof of Eq. (157) is as follows: Noting that the left-hand side of Eq. (157) is manifestly Lorentz invariant (recall Eq. (27)), we may choose \( \Sigma \) to be a constant \( X^0 \)-plane without loss of generality:

\[
N^2 \int_{\Sigma_X} \frac{-2q_\mu \Sigma^\mu}{(2\pi)^d} \int \frac{d^d P}{2E_P} e^{-i(p-q)X^0} e^{i\sigma(P+q)} e^{i\sigma(P+q)} = 2E_p \delta^d(p-q) \tag{158}
\]

We may rewrite the completeness relation (155) in a different fashion:

\[
M^2 \int_{\Sigma_X} \frac{d^d \Sigma^\mu}{(2\pi)^d} \int \frac{d^d P}{2E_P} \langle -2P_\mu | X, P \rangle \langle X, P | \hat{1} \rangle = \hat{1}, \tag{159}
\]

where

\[
M^2 := \frac{1}{N^2} \left[ \frac{K_{d+1}(2\sigma m^2)}{K_{d+1}(2\sigma m^2)} \right] = \frac{K_{d+1}(2\sigma m^2)}{(\sigma \pi)^{d+1} \sqrt{K_{d+1}(2\sigma m^2)}} \tag{160}
\]

To show this, we may sandwich the two sides by \( \langle p | \) and \( | q \rangle \), take the frame where \( \Sigma_X \) becomes a constant \( X^0 \)-plane, and use Eq. (205).\textsuperscript{24}

The completeness (155) on the one-particle subspace \( L^2(\mathbb{R}^d) \) can be naturally generalized to that on the whole Fock space \( \mathcal{H} \) as follows. When we define \( \hat{\Sigma}_{X,P} \) by

\[
\hat{\Sigma}_{X,P} | 0 \rangle := | X, P \rangle, \tag{161}
\]

\textsuperscript{23} In the current on-shell formulation, the free one-particle Hilbert space is spanned within a \( d \)-dimensional spatial hyperplane that is a fixed-time surface in a certain Lorentz frame; On an arbitrary spatial hyperplane \( \Sigma \), integral of the probability density becomes unity, \( \int_{\Sigma} d^d \Sigma^\mu \langle X, P | x \rangle 2i \partial_{\mu} \langle x | X, P \rangle = 1 \); see Eq. (38). It might be interesting to develop an off-shell formulation spanned within the whole enlarged \( D \)-dimensional spacetime and to discuss the uncertainty relation between time and energy more directly there.

\textsuperscript{24} This computation is inspired by Ref. [6].
with mass dimensions $[\hat{A}_{X,P}] = [\{X, P\}] = 0$, we obtain that is,

$$\langle x - X \rangle \cdot P = 0, \quad (x - X)^2 + \sigma^2 m^2 < \left( x^0 - X^0 \right)^2. \quad (168)$$

In a coordinate system $x'$ that is a rest frame for $P$, the cut is along

$$x^0 = X^0, \quad (x' - X')^2 + \sigma^2 m^2 < 0. \quad (169)$$

This is never satisfied and hence we are never on the cut; see also the last paragraph in Appendix B.1.

To cultivate some intuition, we show the case of $\Sigma_X$ being a constant-$X^0$ plane:

$$\hat{\phi}(x) = \frac{2 m^d \left( \frac{\sigma}{\pi} \right)^{d-1}}{\sqrt{2 \pi K_{\frac{d-1}{2}}(2\sigma m^2)}} \int_{\Sigma_X} \frac{d^d X}{(2\pi)^d 2E_P} \frac{K_{\frac{d-1}{2}}(\| \Xi \|)}{\| \Xi \|^{\frac{d-1}{2}}} \left( \frac{1}{\sigma E_P} \right) + i \left( x^0 - X^0 \right) \hat{A}_{X,P} + \text{h.c.} \quad (170)$$

## 6 Summary and discussion

We have proposed a Lorentz-invariant generalization of the Gaussian wave packet. This Lorentz-invariant wave packet has a more natural dependence on the central position $X$ and momentum $P$ than the coherent state in the position–momentum space: The dependence is holomorphic through the variable $X + i \sigma P$ if we further generalize it for a time-like off-shell momentum $P$.

We have obtained the wave function for the Lorentz-invariant wave packet in an closed analytic form, as well as their inner products. The wave function is localized in space but not in time, while its width becomes larger and larger as the time is more and more apart from $X^0$.

We have computed the expectation value and (co)variance of momentum for this state in a closed analytic form, and those of position in the saddle-point approximation. They reduce to the minimum position–momentum uncertainty of the corresponding Gaussian wave packet in the non-relativistic limit. The time–energy uncertainty takes the same minimum value at the leading order in the large width expansion.

We have managed to obtain the completeness relation for these Lorentz-invariant wave packets in a manifestly Lorentz-invariant fashion. It would be interesting to use the complete set of the Lorentz-invariant wave packets instead of the Gaussian ones in the decay and scattering processes ana-
lyzed so far. It would be worth applying to the wave packets in neutrino physics too.

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Appendix A: More on coherent states

We define the displacement operator:

\[ \hat{D}(\alpha) := e^{-\frac{\alpha \hat{a} \dagger - \alpha^* \hat{a}}{2|\alpha|^2}}. \]  

(171)

Note that \( \hat{D}^\dagger(\alpha) = \hat{D}(-\alpha) \). Using the Baker–Campbell–Hausdorff formula,

\[ e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]} , \]

(172)

for the case of \([\hat{A}, \hat{B}]\) being a (commuting) number, we can show that \( \hat{D} \) is unitary, \( \hat{D} \hat{D}^\dagger = \hat{D}^\dagger \hat{D} = 1 \), and that

\[ \hat{D}(\alpha) = e^{-\frac{|\alpha|^2}{4|\lambda|^2}} e^{\frac{\alpha \hat{a} \dagger}{2|\lambda|^2}} e^{\frac{-\alpha^* \hat{a}}{2|\lambda|^2}} , \]

\[ \hat{D}(\alpha) \hat{D}(\beta) = e^{\frac{\beta \hat{a} \dagger - \beta^* \hat{a}}{4|\lambda|^2}} \hat{D}(\alpha + \beta) , \]

(173)

(174)

where we have defined \(|\alpha|^2 := \alpha^* \cdot \alpha = \sum_{i=1}^{d} |\alpha_i|^2 \). We then get

\[ \langle \alpha | \beta \rangle = \langle \varphi | \hat{D}(\alpha) \hat{D}(\beta) | \varphi \rangle \]

\[ = e^{-\frac{|\alpha|^2}{4|\lambda|^2}} \langle \varphi | \hat{D}(\alpha) \hat{D}(\beta) | \varphi \rangle e^{-\frac{|\beta|^2}{2|\lambda|^2}} = e^{-\frac{|\alpha|^2+|\beta|^2}{4|\lambda|^2}} e^{\frac{\alpha^* \hat{a}}{2|\lambda|^2}} . \]

(175)

The ground state of the harmonic oscillator \(|\varphi\rangle\) is given by

\[ \hat{a} |\varphi\rangle = 0 . \]

(176)

That is, \(|\varphi\rangle = |\alpha\rangle\big|_{\alpha=0} \), namely,

\[ \langle \varphi | p \rangle = \frac{(\pi \sigma)}{\hat{a} \hat{a} \dagger} e^{-\frac{p^2}{2\sigma^2}} . \]

(177)

From the commutator

\[ [\hat{a}_i, \hat{D}(\alpha)] = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \hat{a}_i, \left( \frac{\alpha \cdot \hat{a} \dagger - \alpha^* \hat{a}}{2|\lambda|^2} \right)^n \right] \]

\[ = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\alpha_i [\hat{a}_i, \hat{a}_i \dagger]}{2|\lambda|^2} \left( \frac{\alpha \cdot \hat{a} \dagger - \alpha^* \hat{a}}{2|\lambda|^2} \right)^{n-1} \]

\[ = \alpha_i \hat{D}(\alpha) , \]

(178)

we see that \( \hat{a}_i \hat{D}(\alpha) |\varphi\rangle = \alpha_i \hat{D}(\alpha) |\varphi\rangle \), namely,

\[ |\alpha\rangle = \hat{D}(\alpha) |\varphi\rangle \]

(179)

and that the similarity transformation of the annihilation operator results in its displacement:

\[ \hat{D}(\alpha) \hat{a} \hat{D}(\beta) = \hat{a} + \alpha . \]

(180)

In this sense, \(|\alpha\rangle\) is the ground state of the harmonic oscillator displaced by \(\alpha\).

Appendix B: Master integral

We encounter an integral of the form

\[ I(\Xi) := \int \frac{d^d p}{2\pi^d} e^{ip \Xi} \]

(181)

where \( p \) is on-shell and \( \Xi \) is an arbitrary complex \( D \)-vector of dimension \(-1 \). For a massive particle \( p^2 = -m^2 < 0 \), it is more convenient to use the \( D \)-velocity \( u := p/m \) as an integration variable. Hereafter, we always take \( u \) “on-shell”, \( u^2 = -1 \) and \( u^0 = \sqrt{1+u^2} \), unless otherwise stated. Let us define

\[ I(\Xi) := \int \frac{d^d u}{2iu^0} e^{iu \Xi} = \int d^D u \delta(u^2 + 1) \theta(u^0) e^{iu \Xi} , \]

(182)
where $u$ is on-shell and off-shell for the first and second integrals, respectively, and $\Xi$ is a dimensionless complex $D$-vector. Trivially substituting $\Xi = m \bar{\Xi}$, we get

$$i(\bar{\Xi}) = m^{d-1} I(m \bar{\Xi}).$$

(183)

So far we have not put any kind of on-shell condition on $\Xi$, and hence

$$\partial \| \Xi \| / \partial \Xi^\mu = - \Xi_{\mu} / \| \Xi \|,$$

(184)

where $\| \Xi \| := \sqrt{-\Xi^2} = \sqrt{(\Xi^0)^2 - \Xi^2}$ as given in the main text.

We write $\Xi = : P + i Q$, and $\Xi = : Q$, which later will correspond to some momentum and position, respectively:

$$\Xi = P + i Q.$$

(185)

Trivially, $\Xi^2 = (P + i Q)^2 = P^2 + 2i P \cdot Q - Q^2$.

## B.1 Evaluation of master integral

We focus on the case of $P$ being timelike, $P^2 = -(P^0)^2 + P^2 < 0$, and future-oriented, $P^0 > 0$, so that there exists a (proper orthochronous) Lorentz transformation $\Lambda$ to the “rest frame” $\bar{P} = (\bar{P}^0, 0)$ with $\bar{P}^0 = \|P\| > 0$ such that $\Lambda P = \bar{P}$. For a given $P$, concrete form of $\Lambda$ is, in matrix notation,

$$\Lambda = \begin{bmatrix} U^0 & -U^t \\ -\bar{U} \bar{\tau} + (U^0 - 1) \bar{U} \bar{\tau}^t \end{bmatrix},$$

(186)

where $U := P / \|P\|$, $\bar{U} := U / \|U\|$, $\bar{\tau}$ is the $d$-dimensional unit matrix, and $U^0 = \sqrt{1 + \bar{U}^2}$; see e.g. Ref. [28]. We write $\bar{\Xi} := \Lambda Q$ and $\bar{\Xi} := : P + i \bar{Q}$. Note that $\bar{P} = 0$ implies $\bar{\Xi} = i \bar{Q}$. On the other hand, we leave $Q$ to be an arbitrary real $D$ vector.

We change the integration variable to $\tilde{u} := \Lambda u$. Using the Lorentz invariance of the integration measure etc. as well as $(\Lambda^{-1} \tilde{u}) \cdot \Xi = \tilde{u} \cdot (\Lambda \Xi) = \tilde{u} \cdot \bar{\Xi}$, we get

$$I = \int d^D \tilde{u} \delta(\tilde{u}^2 + 1) \delta(\tilde{u}^0) e^{\sqrt{\bar{\Xi}^2 + \tilde{u}^2}}.$$

(187)

Using $\tilde{u} \cdot \bar{\Xi} = -\tilde{u}^0 \bar{\Xi}^0 + \tilde{u} \cdot \bar{\Xi} = -\tilde{u}^0 \bar{\Xi}^0 + i \tilde{u} \cdot \bar{\Xi}$ and renaming $\tilde{u}$ by $u$, we get

$$I = \int d^D u \frac{u^{d-1} u^0}{2 \sqrt{1 + u^2 e^{\sqrt{\bar{\Xi}^2 + u^2} + i u \bar{\Xi}}}}$$

$$= \Omega_{d-1} \int_0^\infty \sin^{d-2} \theta \ d \theta / \sqrt{\bar{\Xi}^2 / \Gamma(\frac{d-1}{2}) / \Gamma(\frac{d}{2})} e^{-\sqrt{\bar{\Xi}^2 + u^2} + i u \bar{\Xi} \cos \theta},$$

(188)

where $\Omega_{d-1} = \frac{2 \pi^{d/2}}{\Gamma(\frac{d}{2})}$ is the area of a unit $(d - 1)$-sphere (boundary of unit $d$-ball).

We follow Ref. [23] in the following. The angular integral reads

$$I = \int_0^\pi \sin^{d-2} \theta \ d \theta / \sin \theta \sqrt{\bar{\Xi}^2 / \sqrt{\bar{\Xi}^2 + u^2} + i u \bar{\Xi} \cos \theta}$$

$$= \sqrt{\pi} \Gamma(\frac{d-1}{2}) \frac{2}{\sqrt{\bar{\Xi}^2 / \Gamma(\frac{d}{2})}} \left( \frac{2}{u \bar{\Xi}} \right) \int_0^\infty \left( \bar{\Xi}^2 - 1 \right) J_{d-2}(u \bar{\Xi}) \ e^{e^{-u \bar{\Xi}}},$$

(189)

where $J$ is the Bessel function of the first kind. (For $d = 3$, the right-hand side comes back to the familiar form $2 \sin(u \bar{\Xi}) / u \bar{\Xi}$.) Now

$$I = \frac{\Omega_{d-1} \Gamma(\frac{d}{2})}{2} \left( \frac{2}{\bar{\Xi}} \right) \int_0^\infty \left( \bar{\Xi}^2 - 1 \right) J_{d-2}(u \bar{\Xi}) \ e^{e^{-u \bar{\Xi}}},$$

(190)

where $\varepsilon := \sqrt{1 + u^2}$ is a rescaled energy. We use the second formula of Eq. (6.645) in Ref. [29]:

$$\int_0^\infty dx \left( x^2 - 1 \right)^{\frac{d}{2}} \varepsilon^{\alpha} J_{\nu}(\beta \sqrt{x^2 - 1})$$

$$= \frac{\sqrt{\pi}}{\Gamma(\frac{d}{2})} \left( \frac{\alpha^2 + \beta^2}{\beta^2} \right)^{\frac{d-1}{2}} K_{d-1}(\sqrt{\alpha^2 + \beta^2}).$$

(191)

applicable for $\Re \alpha > 0$. Setting $\alpha = \bar{\Xi}^0$, $\beta = |\bar{\Xi}|$, and $\nu = \frac{d-2}{2}$, we get

$$I(\Xi) = (2\pi)^{\frac{d-1}{2}} \frac{K_{d-1}(\|\Xi\|)}{\|\Xi\|^{\frac{d-1}{2}}}$$

(192)

where we used

$$\bar{\Xi}^0 + \bar{\Xi}^2 = (\bar{P}^0)^2 + 2i \bar{P}^0 \bar{\Xi}^0 - (\bar{P}^0)^2 + \bar{\Xi}^2$$

$$= -\bar{P}^2 - 2i \bar{P}^0 \cdot \bar{Q} + \bar{\Xi}^2$$

$$= -\bar{\Xi}^2 = -\bar{\Xi}^2 = \|\Xi\|^2.$$

(193)

The limit $\|\Xi\| \to \infty$ is

$$I \to (2\pi)^{\frac{d-1}{2}} \sqrt{\frac{\pi}{2}} \frac{e^{-\|\Xi\|}}{\|\Xi\|^\frac{d-1}{2}} \left( 1 + O\left( \frac{\|\Xi\|}{\|\Xi\|} \right) \right).$$

(194)
whereas $\| \Xi \| \to 0$ gives

$$\mathcal{I} \to (2\pi)^{d-1} \frac{2^{d-2} \Gamma(\frac{d-1}{2})}{\| \Xi \|^{d-1}} \left( 1 + O(\| \Xi \|) + O(\ln \| \Xi \|) \right).$$

(195)

Recall that we are assuming $d \geq 2$.

Throughout this paper, we choose to place a branch-cut for a square root, say $\sqrt{z}$, on the negative real axis of $z$-plane: For $-\pi < \theta < \pi$ and $r \geq 0$,

$$\sqrt{r e^{i\theta}} := \sqrt{re^{i\theta/2}}.$$  (196)

In particular we may use the following limit for $y \to 0$ under $x > 0$:

$$-x - iy \to -i \text{ sgn}(y) \sqrt{x} \left( 1 + i \frac{y}{2x} + \cdots \right).$$  (197)

Then for Eq. (93), the condition on the argument to be on the real axis is

$$0 \leq \Im \left( -\Xi^2 \right) = \Im \left( -\bar{\Xi}^2 \right) = 2\bar{\Xi}^0 \bar{\Xi}^0.$$  (198)

As $\bar{\Xi}^0 > 0$, we see that $\bar{\Xi}^0 \Xi^0 = 0$ is it. However, the real part of the argument on the real axis ($\bar{\Xi}^0 = 0$) is positive:

$$\Re \left( -\Xi^2 \right) = \Re \left( -\bar{\Xi}^2 \right) = \left( \bar{\Xi}^0 \right)^2 + \Xi^2 > 0.$$  (199)

To summarize, no ambiguity arises from the branch cut as long as $\mathcal{P}$ is timelike: $\mathcal{P}^2 < 0$. More in general, we may perform analytic continuation of the result (93) so long as $\Im \left( -\Xi^2 \right) \propto \mathcal{P} \cdot Q \neq 0$ or $\Re \left( -\Xi^2 \right) = \mathcal{Q}^2 - \mathcal{P}^2 > 0$. On the other hand, possible non-triviality arises when $\mathcal{Q}^2 < \mathcal{P}^2$ ($< 0$) in the limit $\mathcal{P} \cdot Q \to 0$:

$$-\Xi^2 = -\mathcal{P}^2 - 2i\mathcal{P} \cdot Q + \Xi^2 \to -i \text{ sgn}(\mathcal{P} \cdot Q) \sqrt{\mathcal{P}^2 - \Xi^2} \left( 1 + i \frac{\mathcal{P} \cdot Q}{\mathcal{P}^2 - \Xi^2} + \cdots \right).$$  (200)

B.2 Derivative of master integral

We define

$$\mathcal{I}^{\mu_1 \cdots \mu_n}(\Xi) := \frac{\partial^n}{\partial \Xi_{\mu_1} \cdots \partial \Xi_{\mu_n}} \mathcal{I}(\Xi).$$  (201)

We note that

$$\mathcal{I}^{\mu_1 \cdots \mu_n}(\Xi) = \int \frac{d^d u}{2u^0} e^{u \cdot \Xi} u^{\mu_1} \cdots u^{\mu_n}$$

$$= \int d^D u \delta \left( u^2 + 1 \right) \theta \left( u^0 \right) e^{u \cdot \Xi} u^{\mu_1} \cdots u^{\mu_n}.$$  (202)

where $u$ is on-shell and off-shell in the first and second integrals, respectively. Using

$$\frac{d\mathcal{I}}{d \| \Xi \|^2} = \left( 2\pi \right)^{d-1} \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}},$$

$$\frac{d^2 \mathcal{I}}{d \| \Xi \|^2} = \left( 2\pi \right)^{d-1} \left[ \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}} + \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}} \right],$$  (203)

and

$$\frac{\partial \| \Xi \|}{\partial \Xi_\mu} = -\frac{\Xi_\mu}{\| \Xi \|}, \quad \frac{\partial^2 \| \Xi \|}{\partial \Xi_\mu \partial \Xi_\nu} = -\frac{1}{\| \Xi \|} \left( \eta_{\mu \nu} - \frac{\Xi_\mu \Xi_\nu}{\Xi^2} \right),$$  (204)

we obtain

$$\mathcal{I}^{\mu} = \frac{\partial \mathcal{I}}{\partial \Xi_\mu} = \left( 2\pi \right)^{d-1} \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}} \Xi^\mu,$$  (205)

$$\mathcal{I}^{\mu \nu} = \frac{\partial^2 \mathcal{I}}{\partial \Xi_\mu \partial \Xi_\nu} = \frac{\partial^2 \| \Xi \|}{\partial \Xi_\mu \partial \Xi_\nu} \frac{d\mathcal{I}}{d \| \Xi \|}$$

$$+ \frac{\partial \| \Xi \|}{\partial \Xi_\mu} \frac{\partial \| \Xi \|}{\partial \Xi_\nu} \frac{d^2 \mathcal{I}}{d \| \Xi \|^2}$$

$$= \left( 2\pi \right)^{d-1} \left[ \eta_{\mu \nu} \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}} - \frac{\Xi_\mu \Xi_\nu}{\Xi^2} \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}} \right].$$  (206)

By construction, we have the identity

$$\eta_{\mu \nu} \mathcal{I}^{\mu \nu} = -\mathcal{I},$$  (207)

namely,

$$(d + 1) \frac{K_{d+1} (\| \Xi \|)}{\| \Xi \|^{{d+1}}} - K_{d+1} (\| \Xi \|) = -K_{d+1} (\| \Xi \|),$$  (208)

which is exactly the identity that the modified Bessel function satisfies.

B.3 Integral of master integral

For later convenience, we define

$$\mathcal{I}^{\mu_1 \cdots \mu_n}_{(a)}(\Xi) := \int \frac{d^d u}{2u^0} e^{u \cdot \Xi} u^{\mu_1} \cdots u^{\mu_n}$$  (209)

for an arbitrary complex $D$-vector $\Xi$ that is not necessarily on-shell, while $u$ as always is: $u^0 = \sqrt{1 + u^2}$. This integral
is Lorentz-covariant when and only when $n = 0$. Note that $T^{\mu_1 \cdots \mu_n} (\Xi) = T^{\mu_1 \cdots \mu_n} (\Xi)$ and $I_{(\Theta)} (\Xi) = I (\Xi)$.

We note that

$$I_{(\Theta)} (\Xi) = \frac{\partial^\ell}{\partial \Xi_{i_1} \cdots \partial \Xi_{i_\ell}} I (\Xi),$$

where indices are not summed.

### B.3.1 Saddle-point method

We compute $I_{(\Theta)} (\Xi)$ in the large $\| \Xi \|$ expansion. Concretely, we compute the following integral using the saddle-point method in the limit $\lambda \gg 1$:

$$I_{(\Theta)} (\Xi) = \int \frac{d^4 u}{2\mu_0^3} e^{u \cdot (\Theta) / \mu_0} = \int \frac{d^4 u}{2} e^{F},$$

where

$$F := \lambda u \cdot \Theta - (n + 1) \ln \mu_0.$$ 

Note that $\Theta$ is “off-shell” in the sense that $\Theta^0$ is treated as an independent variable. For reference, we list the derivatives of exponent before setting to the saddle point:

$$\frac{\partial F}{\partial u'} = \lambda \left( \Theta_i - \frac{u_i}{u'^0} \Theta^0 \right) - (n + 1) \frac{u_i}{(u'^0)^2},$$

$$\frac{\partial^2 F}{\partial u'^0 \partial u'} = -\delta_{ij} \left( \frac{\Theta^0}{u'^0} + \frac{n + 1}{(u'^0)^2} \right) + u_{i,j} u_{i,j},$$

$$\frac{\partial^3 F}{\partial u'^0 \partial u' \partial u'} = \delta_{ij,k} u_{i,k} + \delta_{i} u_{j,k} + \delta_{j} u_{i,k},$$

$$\frac{\partial^4 F}{\partial u'^0 \partial u' \partial u' \partial u'} = \delta_{i,j,k,l} u_{i,j,k,l}.$$ 

To obtain the saddle point, we solve

$$\frac{\partial F}{\partial u'} = \lambda \left( \Theta_i - \frac{u_i}{u'^0} \Theta^0 \right) - (n + 1) \frac{u_i}{(u'^0)^2} = 0.$$

We put an ansatz

$$u_i = \Theta_i - \frac{C n}{\lambda n}$$

to get the solution

$$C_0 = \frac{1}{\| \Theta \|}, \quad C_1 = -\frac{n + 1}{\| \Theta \|^2}, \quad C_2 = \frac{(n + 1)^2}{2 \| \Theta \|^3}, \quad C_3 = -\frac{(n + 1)^3}{\| \Theta \|^4},$$

etc. Then, at the saddle point,

$$e^{F_*} = e^{-\lambda \| \Theta \|} \left( \frac{\| \Theta \|}{\Theta^0} \right)^{n+1} \left( 1 + \frac{(n + 1)^2}{2 \lambda \| \Theta \|^2} \Theta^0 + \cdots \right).$$

Around the saddle point, we expand the integrand for large $\lambda$:

$$e^{F_*} = e^{F_* + \frac{1}{2} \Delta u_i M_{ij} \Delta u_j} \left[ 1 + \frac{1}{3!} \frac{\partial^3 F_*}{\partial u'^i \partial u'^j \partial u'^k} \Delta u_i \Delta u_j \Delta u_k \right. +$$

$$+ \frac{1}{4!} \frac{\partial^4 F_*}{\partial u'^i \partial u'^j \partial u'^k \partial u'^\ell} \Delta u_i \Delta u_j \Delta u_k \Delta u_\ell$$

$$\left. + \frac{1}{2 \lambda} \frac{\partial^4 u_*}{\partial u'^i \partial u'^j \partial u'^k \partial u'^\ell} \Delta u_i \Delta u_j \Delta u_k \right] + \cdots,$$

where we have shifted the variables as $\Delta u := u - u_*$. We have neglected all terms of order $1/\lambda^2$, with $\Delta u$ being counted as $1/\sqrt{\lambda}$. The derivatives at the saddle point are

$$\left. \frac{\partial^2 F_*}{\partial u'^i \partial u'^j} \right|_{u_*} = -\lambda \| \Theta \| \left( \delta_{ij} - \frac{\Theta_i \Theta_j}{\Theta^0} \right)$$

$$- \lambda \| \Theta \| \delta_{ij} \left( 1 + \frac{n + 1}{\lambda \| \Theta \|} + \cdots \right)$$

$$= -\lambda \| \Theta \| \delta_{ij} \left( 1 + \frac{n + 1}{\lambda \| \Theta \|} + \cdots \right).$$

28 Without large $\lambda$ expansion, we may directly put $u' = C \Theta'$:

$$\lambda \left( 1 - C \frac{\Theta^0}{\sqrt{1 + C^2 \Theta^2}} \right) - (n + 1) \frac{C}{1 + C^2 \Theta^2} = 0.$$
\[
\frac{\partial^3 F}{\partial u^i \partial u^j \partial u^k} = \left( \delta_{ij} \delta_{k\ell} + \delta_{jk} \delta_{i\ell} + \delta_{ki} \delta_{j\ell} \right) \left( \frac{\lambda \|\Theta\|^3}{(\Theta^0)^3} + \cdots \right) - \left( \delta_{ij} \delta_{k\ell} + \delta_{jk} \delta_{i\ell} + \delta_{ki} \delta_{j\ell} \right) \left( \frac{\lambda \|\Theta\|^3}{(\Theta^0)^3} + \cdots \right) + \Theta_{ij} \Theta_{k\ell} \left( 15 \lambda \|\Theta\|^3 \left(\Theta^0\right)^6 + \cdots \right)
\]

Let \( M \) be the Hessian at the saddle point:
\[
M_{ij} := \left. \frac{\partial^2 F}{\partial u^i \partial u^j} \right|.
\]
We write the eigenvectors and eigenvalues of \( M \) as
\[
M V^{(n)} = -\lambda^{(n)} V^{(n)},
\]
in which \( n \) is not summed. Then we may diagonalize \( M \) as
\[
R^t M R = \hat{M}
\]
where
\[
\hat{M} := \begin{bmatrix}
-\lambda^{(1)} \\
\vdots \\
-\lambda^{(d)}
\end{bmatrix}, \quad R := \begin{bmatrix} V^{(1)} & \cdots & V^{(d)} \end{bmatrix}.
\]

Here, \( R \) is a complex orthogonal matrix \( R^t R = 1 \).

Now we may change the variables as
\[
\frac{1}{2} \Delta u_i M_{ij} \Delta u_j = \frac{1}{2} \tilde{\Delta} u_i \tilde{M}_{ij} \tilde{\Delta} u_j = -\frac{\lambda^{(n)}}{2} \tilde{\Delta} u_n^2,
\]
with
\[
\Delta u_i = R_{ij} \tilde{\Delta} u_j.
\]

Then we obtain
\[
\frac{\partial^3 F_*}{\partial u^i \partial u^j \partial u^k} \Delta u_i \Delta u_j \Delta u_k = \frac{1}{3!} \tilde{\Delta} \Delta \Delta u_i \Delta u_j \Delta u_k
\]
\[
= \frac{1}{3!} \tilde{\Delta} \Delta \Delta u_i \Delta u_j \Delta u_k,
\]
\[
\frac{\partial^4 F_*}{\partial u^i \partial u^j \partial u^k \partial u^l} \Delta u_i \Delta u_j \Delta u_k \Delta u_l
\]

where
\[
\frac{\partial^3 F_*}{\partial u^i \partial u^j \partial u^k} = \left( \delta_{ij} \delta_{k\ell} + \delta_{jk} \delta_{i\ell} + \delta_{ki} \delta_{j\ell} \right) \left( \frac{\lambda \|\Theta\|^3}{(\Theta^0)^3} + \cdots \right) \times \left( \frac{\lambda \|\Theta\|^3}{(\Theta^0)^3} + \cdots \right) + \Theta_{ij} \Theta_{k\ell} \left( 15 \lambda \|\Theta\|^3 \left(\Theta^0\right)^6 + \cdots \right),
\]

Because our Hessian takes the form
\[
M_{ij} = A \delta_{ij} + B \Theta_i \Theta_j,
\]
with
\[
A = -\lambda \|\Theta\| \left( 1 + \frac{n}{\lambda \|\Theta\|} + \cdots \right),
\]
\[
B = \lambda \|\Theta\| \left( 1 + \frac{n}{\lambda \|\Theta\|} \left(\Theta^0\right)^3 + \cdots \right).
\]
we obtain
\[
M_{ki} R_{kj} = A \delta_{ij} + B \tilde{\Theta}_i \tilde{\Theta}_j,
\]
where \( \tilde{\Theta}_i := \Theta_i R_{ji}, \) that is, \( \Theta_i = R_{ij} \tilde{\Theta}_j. \) In particular,
\[
\tilde{\Theta}_k = \begin{cases} 0 & (k \neq d), \\ \sqrt{\Theta^2} & (k = d). \end{cases}
\]

Then we get
\[
\frac{\partial^3 F_*}{\partial u^i \partial u^j \partial u^k} \Delta u_i \Delta u_j \Delta u_k
\]
\[
\begin{align*}
&= 3 \left( \tilde{\Delta} u_\perp^2 + \tilde{\Delta} u_{\|}^2 \right) \tilde{\Delta} u_{\|} \sqrt{\Theta^2} \left( \lambda \frac{\| \Theta \|^2}{\Theta^0} + \cdots \right) \\
&\quad + \tilde{\Delta} u_{\|}^4 (\Theta^0)^2 \left( -3 \lambda \frac{\| \Theta \|^3}{(\Theta^0)^4} + \cdots \right), \\
&= 3 \left( \tilde{\Delta} u_\perp^2 + \tilde{\Delta} u_{\|}^2 \right) \left( \lambda \frac{\| \Theta \|^3}{\Theta^0} + \cdots \right) \\
&\quad - 6 \left( \tilde{\Delta} u_\perp^2 + \tilde{\Delta} u_{\|}^2 \right) \tilde{\Delta} u_{\|}^2 (\Theta^0)^2 \left( \frac{3 \lambda}{\Theta^0} + \cdots \right) \\
&\quad + \tilde{\Delta} u_{\|}^4 (\Theta^0)^2 \left( \frac{15 \lambda}{\Theta^0} \right) + \cdots
\end{align*}
\]
Keeping the lowest order terms for large $\lambda$ in Eq. (248), we get

\begin{align}
\int d^d \tilde{u} e^{ \frac{-i \delta}{2} \sqrt{\| \tilde{u} \|^2 - \Theta^2} } \frac{\partial^4 F_{\lambda}}{\partial u^4 \partial u^j \partial u^k} \tilde{u}_a \tilde{u}_j \tilde{u}_k \tilde{u}_\ell \\
= \left( \frac{2\pi}{\lambda \| \Theta \|} \right)^d \frac{3\Theta^0}{\lambda} (d + 2) \left( \frac{d + 4}{\Theta^0} - \frac{4}{\| \Theta \|^2} \right) + \ldots,
\end{align}

(252)

\begin{align}
\int d^d \tilde{u} e^{ \frac{-i \delta}{2} \sqrt{\| \tilde{u} \|^2 - \Theta^2} } \left( \frac{\partial^3 F_{\lambda}}{\partial u^3 \partial u^j \partial u^k} \tilde{u}_a \tilde{u}_j \tilde{u}_k \tilde{u}_\ell \right)^2 \\
= \left( \frac{2\pi}{\lambda \| \Theta \|} \right)^d 9(d + 2)(d + 4) \frac{\Theta^2}{\| \Theta \|^2} \frac{1}{\lambda \Theta^0} + \ldots.
\end{align}

(253)

To summarize,

\begin{align}
I_{(n)} = \frac{1}{2} \left( \frac{2\pi}{\lambda \| \Theta \|} \right)^d e^{-\lambda \| \Theta \|} \left( \frac{\| \Theta \|}{\Theta^0} \right)^n \\
\times \left[ 1 + \frac{1}{\lambda \| \Theta \|} \left( \frac{d (d - 2)}{8} \\
+ n \left( d + n + 1 \right) \left( \frac{\Theta^2}{\Theta^0} \right) \right) + \ldots \right],
\end{align}

(254)

and hence

\begin{align}
\frac{1}{I_{(n)}} \frac{\partial}{\partial \lambda} I_{(n)} \\
= \frac{\Theta_j}{\| \Theta \|} \left( \frac{\| \Theta \|}{\Theta^0} \right)^n \left[ 1 + \frac{1}{2\lambda \| \Theta \|} \left( d - n (d + 2) + n (n + 1) \left( \frac{\Theta^2}{\Theta^0} \right) \right) + \mathcal{O} \left( \frac{1}{\lambda^2} \right) \right],
\end{align}

(255)

\begin{align}
\frac{1}{I_{(n)}} \frac{\partial^2}{\partial \lambda^2} I_{(n)} \\
= \left( \frac{\| \Theta \|}{\Theta^0} \right)^n \left[ \delta_{ij} + \Theta_i \Theta_j \left( \frac{d + 1}{\| \Theta \|^2} \right) \\
- \frac{n}{2} \left( d + 4 - (n + 1) \left( \frac{\Theta^2}{\Theta^0} \right) \right) \right] + \mathcal{O} \left( \frac{1}{\lambda^2} \right),
\end{align}

(256)

where we used

\begin{align}
\frac{\partial}{\partial \lambda} \| \Theta \| = \frac{\partial}{\partial \lambda} \left( \frac{\Theta^0}{\Theta^0} \right) - \Theta^0 = \Theta^0.
\end{align}

(257)

B.3.2 Non-relativistic expansion without using saddle-point method

Instead of using the saddle-point method, we may obtain the integral (209) by the non-relativistic expansion, which provides a non-trivial consistency check.

In the non-relativistic limit $\Re \Xi^0 \gg \| \Xi \| \geq 0$, the dominant contribution to the integral would be from the non-relativistic velocity $|u| \ll 1$:

\begin{align}
I_{(n)}(\Xi) = \int \frac{d^d u}{2 \Theta^0} e^{u \Xi} \frac{1}{(u^0)^n} \\
= \int \frac{d^d u}{2 \Theta^0} e^{u \Xi} \left( 1 - \frac{n}{2} u^2 + n (n + 2) \left( \frac{u^2}{2} \right) + \ldots \right) \\
= I(\| \Xi \|) - \frac{n}{2} \frac{\partial}{\partial \Xi^i} I(\| \Xi \|) \\
+ \frac{n (n + 2)}{8} \frac{\partial^4}{\partial \Xi^i \partial \Xi^j \partial \Xi^k \partial \Xi^\ell} I(\| \Xi \|) + \ldots \\
= (2\pi)^{d/2} K_{\frac{d+1}{2}} (\| \Xi \|) \left[ \frac{\| \Xi \|}{\| \Xi \|^2} \right] \\
+ \frac{\| \Xi \|}{\| \Xi \|^2} K_{\frac{d+1}{2}} (\| \Xi \|) + \ldots,
\end{align}

(258)

where we used

\begin{align}
\frac{\partial}{\partial \Xi^i} \frac{\partial}{\partial \Xi^j} = - \frac{\Xi_j}{\| \Xi \|}, \quad \frac{\partial^2}{\partial \Xi^i \partial \Xi^j} = - \delta_{ij} - \frac{\Xi_j \Xi_i}{\| \Xi \|^2}.
\end{align}

(259)

In the above, the $\Xi^0$ are written in terms of $\| \Xi \|$ and $\Xi$.

Now we show results in the non-relativistic expansion with large $\| \Xi \|$, leaving the overall function that cancels out in $\frac{1}{I_{(n)}} \frac{\partial}{\partial \lambda} I_{(n)}$, etc.:

\begin{align}
I_{(n)} = (2\pi)^{d/2} \frac{K_{\frac{d+1}{2}} (\| \Xi \|)}{\| \Xi \|^2} \\
\times \left( 1 - \frac{dn}{2 \| \Xi \|} + \ldots \right),
\end{align}

(260)

\begin{align}
\frac{\partial}{\partial \Xi^i} I_{(n)} \\
= (2\pi)^{d/2} \frac{K_{\frac{d+1}{2}} (\| \Xi \|)}{\| \Xi \|^2} \frac{\Xi_i}{\| \Xi \|^2} \\
\times \left( 1 + \frac{dn}{2 \| \Xi \|} + \ldots \right),
\end{align}

(261)

\begin{align}
\frac{\partial^2}{\partial \Xi^i \partial \Xi^j} I_{(n)} \\
= (2\pi)^{d/2} \frac{K_{\frac{d+1}{2}} (\| \Xi \|)}{\| \Xi \|^2} \frac{1}{\| \Xi \|^2} \left[ \delta_{ij} \\
+ \frac{1}{\| \Xi \|} \left( \frac{dn}{2} \delta_{ij} + \Xi_j \Xi_i \right) + \ldots \right].
\end{align}

(262)
As a cross check, we put $\Sigma = \lambda \Theta$ and take the saddle-point limit for large $\lambda$:

\[
\frac{1}{\mathcal{I}(\Theta)} \frac{\partial \mathcal{I}(\Theta)}{\lambda \partial \Theta^j} = \frac{\Theta_i}{\|\Theta\|} \left[ 1 + \frac{d - n (d + 2)}{2\lambda \|\Theta\|} + \mathcal{O} \left( \frac{1}{\lambda^2} \right) \right],
\]

(263)

\[
\frac{1}{\mathcal{I}(\Theta)} \frac{\partial^2 \mathcal{I}(\Theta)}{\lambda^2 \partial \Theta^i \partial \Theta^j} = \frac{\Theta_i \Theta_j}{\|\Theta\|^2} + \frac{1}{\lambda \|\Theta\|} \left( \delta_{ij} + \frac{\Theta_i \Theta_j}{\|\Theta\|^2} \left( d + 1 - \frac{n}{2} (d + 4) \right) \right) + \mathcal{O} \left( \frac{1}{\lambda^2} \right).
\]

(264)

We can confirm that these results coincide with the saddle-point ones (255) and (256) if we take the NR limit $\frac{\mathcal{I}(\Theta)}{\Theta^i} \to 1$ and $-\frac{\Theta^i}{\Theta^j} \to 0$ there.

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