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Particle decay in Gaussian wave-packet formalism revisited

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We derive Fermi's golden rule in the Gaussian wave-packet formalism of quantum field theory, proposed by Ishikawa, Shimomura, and Tobita, for particle decay within a finite time interval. We present a systematic procedure to separate the bulk contribution from those of time boundaries, while manifestly maintaining the unitarity of the S-matrix, unlike the proposal by Stueckelberg in 1951. We also revisit the suggested deviation from the golden rule and clarify that it indeed corresponds to the boundary contributions, though their physical significance is yet to be confirmed.

Subject Index B30

1. Introduction

Strictly speaking, the S-matrix in quantum field theory is defined only by using wave packets; see any textbook, e.g., Refs. [1,2]. The derivation of a physical quantity, such as a decay rate, in terms of plane waves is "actually more a mnemonic than a derivation" [2].

Ishikawa and Shimomura have proposed a formulation of a free Gaussian wave packet in relativistic quantum field theory [3]; see also Refs. [4–7] for earlier related works. Ishikawa and Tobita have developed a systematic method to approximate the S-matrix in various limits in the Gaussian wave-packet formalism [8–10]; further development has been made by themselves and Tajima to include the photon state [11]. The authors have claimed that there can be a deviation from Fermi's golden rule if we consider an S-matrix with finite time interval [8–11].

Stueckelberg correctly pointed out in 1951 that the plane-wave S-matrix with finite time interval exhibits an extra ultraviolet (UV) divergence coming from the interaction point at the boundary in time [12]. In order to remove it within the plane-wave formalism, a phenomenological factor has been introduced so that the uncertainty of the initial and final times of the process can be taken into account. This has led to the violation of unitarity, and the necessary modification of the S-matrix to cure the pathology has become complicated and rather intractable.

In this paper we revisit the Gaussian wave-packet formalism to *derive* Fermi's golden rule. We separate the bulk effect from the boundary ones, while manifestly maintaining the unitarity. We further show that the possible deviation from Fermi's golden rule claimed in Refs. [8–11] indeed corresponds to the decay at the boundary in time.

For clarity, in Sects. 2–4 we will first spell out our results using an example of the tree-level decay process of a heavy scalar Φ into a pair of light scalars $\phi\phi$ due to the super-renormalizable interaction $\Phi\phi\phi$. In order to show how to generalize our results to include the momentum-dependent factors in

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the interaction and in the wave functions, in Sect. 5 we will then turn to the tree-level decay process of a pseudoscalar φ into a pair of photons due to the non-renormalizable interaction $\varphi F_{\mu\nu}\tilde{F}^{\mu\nu}$. More generalization will be presented in Appendix A.

The paper is organized as follows: In Sect. 2 we review the Gaussian wave-packet formalism for the scalar field. In Sect. 3, we reformulate the Gaussian S-matrix and present a systematic procedure to separate the bulk contribution from the boundary ones. In Sect. 4 we obtain the decay probability and derive Fermi's golden rule. We briefly discuss the boundary effect too. In Sect. 5 we generalize our result to the decay into the diphoton final state. In Sect. 6 we summarize our results. In Appendix A we review the Gaussian wave-packet formalism for the scalar, spinor, and vector. In Appendix B, we show the saddle-point approximation of the Gaussian wave packet in the large-width (plane-wave) expansion. In Appendix C, we show the expressions for the plane-wave and particle limits of the decaying particle and for the decay at rest. In Appendix D we present possible expressions for the boundary limit.

2. Gaussian formalism

We review the Gaussian formalism. As stated above, we consider the decay of a heavy real scalar Φ into a pair of light real scalars $\phi\phi$ by the following interaction:

$$\mathcal{L}_{\text{int}} = -\frac{\kappa}{2}\Phi\phi^2, \tag{1}$$

where κ is a coupling constant of mass dimension unity. The interaction Hamiltonian density is $\mathcal{H}_{\text{int}} = -\mathcal{L}_{\text{int}}$. We write the initial and final momenta as $\boldsymbol{p}_0$ and $\boldsymbol{p}_1, \boldsymbol{p}_2$, respectively. In this section we will let Ψ stand for either Φ or ϕ. We write their masses as m_Φ and m_ϕ and consider the case $m_\Phi > 2m_\phi$.

2.1. Plane-wave S-matrix

First we briefly review the plane-wave computation of the S-matrix. We can expand the free field operator $\hat{\Psi}^{(\text{I})}(x)$ at $x = \left(x^0, \boldsymbol{x}\right) = (t, \boldsymbol{x})$ in the interaction picture in terms of the annihilation and creation operators of planes waves:

$$\hat{\Psi}^{(\text{I})}(x) = \int \frac{d^3\boldsymbol{p}}{\sqrt{2p^0}\,(2\pi)^{3/2}} \left[\hat{a}_\Psi(\boldsymbol{p})\, e^{ip\cdot x} + \hat{a}_\Psi^\dagger(\boldsymbol{p})\, e^{-ip\cdot x}\right]\Bigg|_{p^0 = E_\Psi(\boldsymbol{p})}, \tag{2}$$

where we work in the $(-,+,+,+)$ metric convention and write the kinetic energy

$$E_\Psi(\boldsymbol{p}) := \sqrt{m_\Psi^2 + \boldsymbol{p}^2}. \tag{3}$$

Throughout this paper we use both x^0 and t interchangeably (as well as X^0 and T that appear below).

We define the following free one- and two-particle states:[1]

$$\begin{aligned} |\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{SB})} &= \hat{a}_\Phi^\dagger(\boldsymbol{p}_0)\,|0\rangle\,, \\ |\boldsymbol{p}\rangle_\phi^{(\mathrm{SB})} &= \hat{a}_\phi^\dagger(\boldsymbol{p})\,|0\rangle\,, \\ |\boldsymbol{p}_1,\boldsymbol{p}_2\rangle_{\phi\phi}^{(\mathrm{SB})} &= \frac{1}{\sqrt{2}}\hat{a}_\phi^\dagger(\boldsymbol{p}_1)\,\hat{a}_\phi^\dagger(\boldsymbol{p}_2)\,|0\rangle\,, \end{aligned} \tag{4}$$

where (SB) refers to the time-independent basis state in the Schrödinger picture (see Appendix A.1), which are the eigenstates of the free Hamiltonian:

$$\begin{aligned} \hat{H}_{\mathrm{free}}\,|\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{SB})} &= E_\Phi(\boldsymbol{p}_0)\,|\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{SB})}\,, \\ \hat{H}_{\mathrm{free}}\,|\boldsymbol{p}\rangle_\phi^{(\mathrm{SB})} &= E_\phi(\boldsymbol{p})\,|\boldsymbol{p}\rangle_\phi^{(\mathrm{SB})}\,, \\ \hat{H}_{\mathrm{free}}\,|\boldsymbol{p}_1,\boldsymbol{p}_2\rangle_{\phi\phi}^{(\mathrm{SB})} &= \left(E_\phi(\boldsymbol{p}_1)+E_\phi(\boldsymbol{p}_2)\right)|\boldsymbol{p}_1,\boldsymbol{p}_2\rangle_{\phi\phi}^{(\mathrm{SB})}\,. \end{aligned} \tag{5}$$

In terms of these states, the free field operator in Eq. (2) can also be written as

$$\hat{\Psi}^{(\mathrm{I})}(x) = \int \frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}}\left[\hat{a}_\Psi(\boldsymbol{p})\left({}^{(\mathrm{IB})}_{\ \ \Psi}\langle x\,|\boldsymbol{p}\rangle_\Psi^{(\mathrm{SB})}\right) + \hat{a}_\Psi^\dagger(\boldsymbol{p})\left({}^{(\mathrm{IB})}_{\ \ \Psi}\langle x\,|\boldsymbol{p}\rangle_\Psi^{(\mathrm{SB})}\right)^*\right], \tag{6}$$

where $|x\rangle_\Psi^{(\mathrm{IB})} = e^{i\hat{H}_{\mathrm{free}}t}\,|\boldsymbol{x}\rangle_\Psi^{(\mathrm{SB})}$ is the position basis state in the interaction picture; see Appendix A.2.

Usually, the time-independent in and out states in the Heisenberg picture are defined as the eigenstates of the total Hamiltonian that become close to the free states in Eq. (4) at sufficiently remote past and future in the following sense:[2]

$$e^{-i\hat{H}t}\,|\mathrm{in};\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{H})} \to e^{-i\hat{H}_{\mathrm{free}}t}\,|\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{SB})} \qquad \text{for } t \to T_{\mathrm{in}}\ (\to -\infty), \tag{7}$$

$$e^{-i\hat{H}t}\,|\mathrm{out};\boldsymbol{p}_1,\boldsymbol{p}_2\rangle_{\phi\phi}^{(\mathrm{H})} \to e^{-i\hat{H}_{\mathrm{free}}t}\,|\boldsymbol{p}_1,\boldsymbol{p}_2\rangle_{\phi\phi}^{(\mathrm{SB})} \qquad \text{for } t \to T_{\mathrm{out}}\ (\to \infty), \tag{8}$$

where $\hat{H} = \hat{H}_{\mathrm{free}} + \hat{H}_{\mathrm{int}}$ is the total Hamiltonian. To be more precise, Eqs. (7) and (8) are meaningless in themselves and should rather be understood as follows (see any textbook, e.g., Refs. [1,2]): The in and out states are really defined by *wave packets* such that, for arbitrary smooth and sufficiently fast-decaying functions $g_{\mathrm{in}}(\boldsymbol{p}_0)$ and $g_{\mathrm{out}}(\boldsymbol{p}_1,\boldsymbol{p}_2)$, they satisfy

$$\int d^3\boldsymbol{p}_0\, g_{\mathrm{in}}(\boldsymbol{p}_0)\; e^{-i\hat{H}t}\,|\mathrm{in};\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{H})} \approx \int d^3\boldsymbol{p}_0\, g_{\mathrm{in}}(\boldsymbol{p}_0)\; e^{-i\hat{H}_{\mathrm{free}}t}\,|\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{SB})}\,, \tag{9}$$

[1] The two-particle state is normalized to

$${}^{(\mathrm{SB})}_{\ \ \phi\phi}\langle\boldsymbol{p}_1,\boldsymbol{p}_2\,|\boldsymbol{p}_3,\boldsymbol{p}_4\rangle_{\phi\phi}^{(\mathrm{SB})} = \frac{1}{2}\left[\delta^3(\boldsymbol{p}_1-\boldsymbol{p}_3)\,\delta^3(\boldsymbol{p}_2-\boldsymbol{p}_4) + \delta^3(\boldsymbol{p}_1-\boldsymbol{p}_4)\,\delta^3(\boldsymbol{p}_2-\boldsymbol{p}_3)\right]$$

such that

$$\int d^3\boldsymbol{p}_1 \int d^3\boldsymbol{p}_2\, |\boldsymbol{p}_1,\boldsymbol{p}_2\rangle\langle\boldsymbol{p}_1,\boldsymbol{p}_2| = \hat{1},$$

where $\hat{1}$ is the identity operator in the two-particle subspace.

[2] This can be formally rewritten as the interaction-picture state becoming close to the time-independent Schrödinger basis state as

$$|\mathrm{in};\boldsymbol{p}_0,t\rangle_\Phi^{(\mathrm{I})} \to |\boldsymbol{p}_0\rangle_\Phi^{(\mathrm{SB})} \qquad \text{for } t \to T_{\mathrm{in}}\ (\to -\infty),$$

$$|\mathrm{out};\boldsymbol{p}_1,\boldsymbol{p}_2;t\rangle_{\phi\phi}^{(\mathrm{I})} \to |\boldsymbol{p}_1,\boldsymbol{p}_2\rangle_{\phi\phi}^{(\mathrm{SB})} \qquad \text{for } t \to T_{\mathrm{out}}\ (\to \infty).$$

$$\int d^3\boldsymbol{p}_1\, d^3\boldsymbol{p}_2\, g_{\rm out}(\boldsymbol{p}_1,\boldsymbol{p}_2)\; e^{-i\hat{H}t}\left|{\rm out};\boldsymbol{p}_1,\boldsymbol{p}_2\right\rangle_{\phi\phi}^{(\rm H)} \approx \int d^3\boldsymbol{p}_1\, d^3\boldsymbol{p}_2\, g_{\rm out}(\boldsymbol{p}_1,\boldsymbol{p}_2)\; e^{-i\hat{H}_{\rm free}t}\left|\boldsymbol{p}_1,\boldsymbol{p}_2\right\rangle_{\phi\phi}^{(\rm SB)} \tag{10}$$

as $t \to T_{\rm in}$ $(\to -\infty)$ and $t \to T_{\rm out}$ $(\to \infty)$, respectively.[3]

The S-matrix is defined by

$$S = {}_{\phi\phi}^{(\rm H)}\!\left\langle {\rm out};\boldsymbol{p}_1,\boldsymbol{p}_2 \middle| {\rm in};\boldsymbol{p}_0\right\rangle_{\Phi}^{(\rm H)}. \tag{11}$$

For $T_{\rm in}$ and $T_{\rm out}$ in the sufficiently remote past and future, respectively, one obtains

$$S \approx {}_{\phi\phi}^{(\rm SB)}\!\left\langle \boldsymbol{p}_1,\boldsymbol{p}_2 \right| \hat{U}(T_{\rm out},T_{\rm in}) \left|\boldsymbol{p}_0\right\rangle_{\Phi}^{(\rm SB)}, \tag{12}$$

where

$$\begin{aligned}\hat{U}(T_{\rm out},T_{\rm in}) &:= e^{i\hat{H}_{\rm free}T_{\rm out}}e^{-i\hat{H}(T_{\rm out}-T_{\rm in})}e^{-i\hat{H}_{\rm free}T_{\rm in}}\\ &= {\rm T}\exp\left(-i\int_{T_{\rm in}}^{T_{\rm out}} dt\,\hat{H}_{\rm int}^{(\rm I)}(t)\right),\end{aligned} \tag{13}$$

in which T denotes the time ordering and $\hat{H}_{\rm int}^{(\rm I)}(t) = e^{i\hat{H}_{\rm free}t}\hat{H}_{\rm int}e^{-i\hat{H}_{\rm free}t}$ is the interaction Hamiltonian in the interaction picture.

As is well known, the expression in Eq. (12) is badly divergent when squared, being proportional to the momentum-space delta function $\delta^4(0)$. Also, one needs to insert an infinitesimal imaginary part for the interaction Hamiltonian by hand in order to make the perturbation in Eq. (13) convergent. This is because the overlap between plane waves can never be suppressed no matter how remote a past and future one moves on, which is the reason one needs the wave packets in Eqs. (9) and (10) for complete treatment of the S-matrix. The cluster decomposition never occurs for the infinitely spread plane waves, while it does for properly defined wave packets.

2.2. Gaussian basis

Now we switch from the plane-wave basis to the Gaussian basis. Detailed notations for this subsection can be found in Appendix A.

Instead of the plane-wave expansion of Eq. (2), one may also expand the free field in terms of the annihilation and creation operators of the free Gaussian wave:

$$\hat{\Psi}^{(\rm I)}(x) = \int \frac{d^3\boldsymbol{X}\,d^3\boldsymbol{P}}{(2\pi)^3}\left[f_{\Psi,\sigma;X,\boldsymbol{P}}(x)\,\hat{A}_{\Psi,\sigma}(X,\boldsymbol{P}) + f^*_{\Psi,\sigma;X,\boldsymbol{P}}(x)\,\hat{A}^\dagger_{\Psi,\sigma}(X,\boldsymbol{P})\right], \tag{14}$$

where $\sqrt{\sigma}$ is the width of the wave packet; $\boldsymbol{X}$ is the location of the center at time T (and we write collectively $X = \left(X^0,\boldsymbol{X}\right) = (T,\boldsymbol{X})$, as stated above); and $\boldsymbol{P}$ is its central momentum. We also use the shorthand notation

$$\Pi := (X,\boldsymbol{P}), \qquad \boldsymbol{\Pi} := (\boldsymbol{X},\boldsymbol{P}), \qquad d^6\boldsymbol{\Pi} := \frac{d^3\boldsymbol{X}\,d^3\boldsymbol{P}}{(2\pi)^3}, \tag{15}$$

[3] Strictly speaking, this cannot apply for a decay process. No matter how remote a past we move on to, $t \to T_{\rm in}$ $(\to -\infty)$, we might still find a wave-packet configuration of the final-state particles in which we cannot neglect the interaction at the initial time. To handle this issue, one needs to treat the production process of the parent particle using wave packets too. This will be presented in a separate publication.

so that

$$\hat{\Psi}^{(\mathrm{I})}(x) = \int d^6\mathbf{\Pi}\left[f_{\Psi,\sigma;\Pi}(x)\,\hat{A}_{\Psi,\sigma}(\Pi) + f^*_{\Psi,\sigma;\Pi}(x)\,\hat{A}^\dagger_{\Psi,\sigma}(\Pi)\right]. \tag{16}$$

The explicit form of the coefficient function $f_{\Psi,\sigma;\Pi}$ $(= f_{\Psi,\sigma;X,\boldsymbol{P}})$ is obtained as[4]

$$\begin{aligned} f_{\Psi,\sigma;\Pi}(x) &= \int \frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}}\ {}^{(\mathrm{IB})}_{\ \ \Psi}\langle x\,|\,\boldsymbol{p}\rangle^{(\mathrm{SB})}_\Psi\ {}^{(\mathrm{SB})}_{\ \ \Psi}\langle \boldsymbol{p}\,|\,\Pi\rangle^{(\mathrm{IB})}_\Psi \\ &= \left(\frac{\sigma}{\pi}\right)^{3/4}\int \frac{d^3\boldsymbol{p}}{\sqrt{2p^0}\,(2\pi)^{3/2}} e^{ip\cdot(x-X)-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\bigg|_{p^0=E_\Psi(\boldsymbol{p})}. \end{aligned} \tag{17}$$

Throughout the main text, we abbreviate e.g. $|\sigma;\Pi\rangle$ to $|\Pi\rangle$, in which it is understood that the σ can be different from each other among the in- and out-state particles.

In the large-σ expansion, the leading saddle-point approximation gives

$$f_{\Psi,\sigma;\Pi}(x) \to \left(\frac{\sigma}{\pi}\right)^{3/4}\left(\frac{2\pi}{\sigma}\right)^{3/2}\frac{1}{\sqrt{2P^0}\,(2\pi)^{3/2}} e^{iP\cdot(x-X)-\frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t))^2}{2\sigma}}\bigg|_{P^0=E_\Psi(\boldsymbol{P})}, \tag{18}$$

where

$$\boldsymbol{\Xi}(t) := \boldsymbol{X} + \boldsymbol{V}_\Psi(\boldsymbol{P})\,(t-T) \tag{19}$$

is the location of the center of the wave packet at time t, in which $\boldsymbol{V}_\Psi(\boldsymbol{P}) := \boldsymbol{P}/E_\Psi(\boldsymbol{P})$; see Appendix B.[5] Within this leading-order approximation, the width of the wave pack remains constant in time.

2.3. *Free Gaussian wave-packet states*

Now we can explicitly prepare the free wave-packet states, employed in the right-hand sides of Eqs. (9) and (10),

$$\int d^3\boldsymbol{p}_0\, g_{\mathrm{in}}(\boldsymbol{p}_0)\,|\boldsymbol{p}_0\rangle^{(\mathrm{SB})}_\Phi, \qquad \int d^3\boldsymbol{p}_1\int d^3\boldsymbol{p}_2\, g_{\mathrm{out}}(\boldsymbol{p}_1,\boldsymbol{p}_2)\,|\boldsymbol{p}_1,\boldsymbol{p}_2\rangle^{(\mathrm{SB})}_{\phi\phi}, \tag{20}$$

[4] Note that the two "interaction basis" states are the ones at different times:

$$|x\rangle^{(\mathrm{IB})}_\Psi = e^{i\hat{H}_{\mathrm{free}}t}\,|\boldsymbol{x}\rangle^{(\mathrm{SB})}_\Psi, \qquad |\Pi\rangle^{(\mathrm{IB})}_\Psi = e^{i\hat{H}_{\mathrm{free}}T}\,|\mathbf{\Pi}\rangle^{(\mathrm{SB})}_\Psi,$$

where $t = x^0$ and $T = X^0$ in $\Pi = (X,\boldsymbol{P})$ as always.

[5] $\boldsymbol{\Xi}(t)$ has implicit dependence on m_Ψ, $\boldsymbol{P}$, and X $(=(T,\boldsymbol{X}))$.

respectively, as follows:[6]

$$|\Pi\rangle_{\Phi}^{(\mathrm{SB})} = \hat{A}_{\Phi}^{\dagger}(\Pi)\,|0\rangle\,, \qquad |\Pi_1,\Pi_2\rangle_{\phi\phi}^{(\mathrm{SB})} = \frac{1}{\sqrt{2}}\hat{A}_{\phi}^{\dagger}(\Pi_1)\,\hat{A}_{\phi}^{\dagger}(\Pi_2)\,|0\rangle\,. \tag{21}$$

As stated above, $|\sigma_1,\Pi_1;\sigma_2,\Pi_2\rangle$ is abbreviated to $|\Pi_1,\Pi_2\rangle$ throughout the main text.

2.4. Gaussian S-matrix

Suppose that the interaction in Eq. (1) is negligible at some initial and final times T_{in} and T_{out}. Then we may define the corresponding in and out states, following Eqs. (9) and (10), by[7]

$$\begin{aligned} e^{-i\hat{H}t}\,|\mathrm{in};\Pi_0\rangle_{\Phi}^{(\mathrm{H})} &\approx e^{-i\hat{H}_{\mathrm{free}}t}\,|\Pi_0\rangle_{\Phi}^{(\mathrm{SB})} && (t\to T_{\mathrm{in}}),\\ e^{-i\hat{H}t}\,|\mathrm{out};\Pi_1,\Pi_2\rangle_{\phi\phi}^{(\mathrm{H})} &\approx e^{-i\hat{H}_{\mathrm{free}}t}\,|\Pi_1,\Pi_2\rangle_{\phi\phi}^{(\mathrm{SB})} && (t\to T_{\mathrm{out}}). \end{aligned} \tag{22}$$

Now the Gaussian S-matrix is the inner product between these physical states:

$$S = {}_{\phi\phi}^{(\mathrm{H})}\langle\mathrm{out};\Pi_1,\Pi_2\,|\,\mathrm{in};\Pi_0\rangle_{\Phi}^{(\mathrm{H})}\,. \tag{23}$$

Note that these in and out states become close, in the sense of Eq. (22), to the free states of Eq. (21), which are square-integrable and of finite norm.[8] This is in contrast to the plane-wave S-matrix of Eq. (11), which is the inner product between the states that become close to the plane waves of Eq. (4), which are not square-integrable, not elements of the Hilbert space, and hence not the physical states.[9] Due to this finiteness of the Gaussian S-matrix, the probability for the transition $|\mathrm{in};\Pi_0\rangle_{\Phi}^{(\mathrm{H})} \to |\mathrm{out};\Pi_1,\Pi_2\rangle_{\phi\phi}^{(\mathrm{H})}$ is simply its square: $|S|^2$.[10] There is no need of the hand-waving argument of the momentum delta function $\delta^4(0)$ becoming spacetime volume, etc.

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[6] Explicitly, g_{in} (g_{out}) is a (multiple of independent) free Gaussian wave function(s):

$$g_{\mathrm{in}}(\boldsymbol{p}) = {}_{\Phi}^{(\mathrm{SB})}\langle\boldsymbol{p}\,|\,\Pi\rangle_{\Phi}^{(\mathrm{IB})} = \left(\frac{\sigma}{\pi}\right)^{3/4} e^{-ip\cdot X} e^{-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\Big|_{p^0=E_{\Phi}(\boldsymbol{p})},$$

$$g_{\mathrm{out}}(\boldsymbol{p}_1,\boldsymbol{p}_2) = \prod_{a=1,2} {}_{\phi}^{(\mathrm{SB})}\langle\boldsymbol{p}_a\,|\,\Pi_a\rangle_{\phi}^{(\mathrm{IB})} = \prod_{a=1,2}\left(\frac{\sigma_a}{\pi}\right)^{3/4} e^{-ip_a\cdot X_a} e^{-\frac{\sigma_a}{2}(\boldsymbol{p}_a-\boldsymbol{X}_a)^2}\Big|_{p_a^0=E_{\phi}(\boldsymbol{p}_a)},$$

where each "interaction basis" state is the one at a different time: $|\Pi_A\rangle_{\Psi}^{(\mathrm{IB})} = e^{i\hat{H}_{\mathrm{free}}T_A}\,|\boldsymbol{\Pi}_A\rangle_{\Psi}^{(\mathrm{SB})}$. Note also that we have written the states in Eq. (21) as the time-independent Schrödinger basis states, rather than the interaction basis ones, in the sense that they are independent of the time coordinate t that will appear later in $\hat{H}^{(\mathrm{I})}(t)$, the interaction Hamiltonian in the interaction picture. (Otherwise the two-particle state would have two reference times T_1 and T_2 meaninglessly.)

[7] If we took $T_0 = T_{\mathrm{in}}$ and $T_1 = T_2 = T_{\mathrm{out}}$, we would obtain

$$\begin{aligned} e^{-i\hat{H}t}\,|\mathrm{in};\Pi_0\rangle_{\Phi}^{(\mathrm{H})} &\approx |\boldsymbol{\Pi}_0\rangle_{\Phi}^{(\mathrm{SB})} && (t\to T_{\mathrm{in}}),\\ e^{-i\hat{H}t}\,|\mathrm{out};\Pi_1,\Pi_2\rangle_{\phi\phi}^{(\mathrm{H})} &\approx |\boldsymbol{\Pi}_1,\boldsymbol{\Pi}_2\rangle_{\phi\phi}^{(\mathrm{SB})} && (t\to T_{\mathrm{out}}), \end{aligned}$$

respectively.

[8] Note, however, the issue in footnote 3.

[9] One can extend the notion of Hilbert space to include distributions (such as the Dirac delta "function") by using the rigged Hilbert space, namely the Gelfand triple. In the end, from a given plane-wave S-matrix, one can obtain a physically measurable probability only by convoluting it with wave packets.

[10] So far, we have not considered any boundary effect as we assume here that the interactions are negligible at T_{in} and T_{out}; see also footnote 3.

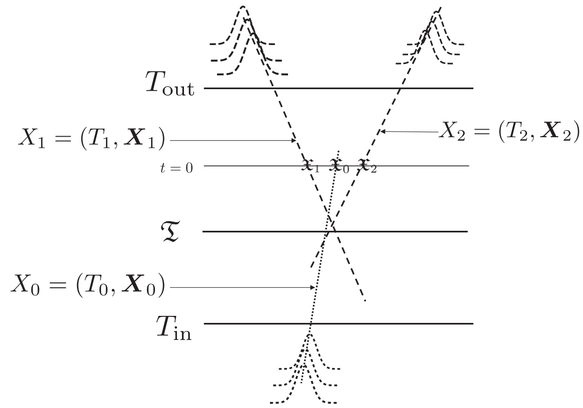


Fig. 1. Schematic figure for a configuration with fixed $\Pi_A = (\boldsymbol{P}_A, X_A)$ with $A = 0, 1, 2$. (The σ_A are kept fixed throughout this paper.) Each wave packet is defined at time T_A as a free Gaussian wave packet centered at $\boldsymbol{X}_A$. Within our leading saddle-point approximation, the widths of the wave packets do not change in time, see Eq. (18), and therefore it does not really matter at which time each wave packet is set to be the free Gaussian wave packet. The wave packets intersect at time $\mathfrak{T}$, around which the interactions occur most. $\mathfrak{X}_A$ is the location of the center of each wave packet at the (arbitrarily chosen) reference time $t = 0$. At time t, the location of the center moves to $\boldsymbol{\Xi}_A(t) = \mathfrak{X}_A + \boldsymbol{V}_A t$.

Using Eq. (22), we get

$$S \approx {}^{\rm (SB)}_{\phi\phi}\langle \Pi_1, \Pi_2 | \, \hat{U}(T_{\rm out}, T_{\rm in}) \, | \Pi_0 \rangle^{\rm (SB)}_{\Phi} . \tag{24}$$

At the first order in the Dyson series of Eq. (13),

$$\hat{U}(T_{\rm out}, T_{\rm in}) = 1 - i \int_{T_{\rm in}}^{T_{\rm out}} dt \int d^3\boldsymbol{x} \, \hat{\mathcal{H}}^{\rm (I)}_{\rm int}(x) + \cdots , \tag{25}$$

the S-matrix becomes

$$\begin{aligned} S &= i \int_{T_{\rm in}}^{T_{\rm out}} dt \int d^3\boldsymbol{x} \; {}^{\rm (SB)}_{\phi\phi}\langle \Pi_1, \Pi_2 | \, \hat{\mathcal{L}}^{\rm (I)}_{\rm int}(x) \, | \Pi_0 \rangle^{\rm (SB)}_{\Phi} \\ &= \frac{i\kappa}{2} \int_{T_{\rm in}}^{T_{\rm out}} dt \int d^3\boldsymbol{x} \; {}^{\rm (SB)}_{\phi\phi}\langle \Pi_1, \Pi_2 | \, \hat{\phi}^{\rm (I)}(x) \, \hat{\phi}^{\rm (I)}(x) \, |0\rangle \; \langle 0 | \, \hat{\Phi}^{\rm (I)}(x) \, | \Pi_0 \rangle^{\rm (SB)}_{\Phi} \\ &= \frac{i\kappa}{\sqrt{2}} \int_{T_{\rm in}}^{T_{\rm out}} dt \int d^3\boldsymbol{x} f^*_{\phi,\sigma_1;\Pi_1}(x) \, f^*_{\phi,\sigma_2;\Pi_2}(x) \, f_{\Phi,\sigma_0;\Pi_0}(x) \, . \end{aligned} \tag{26}$$

3. Gaussian S-matrix: separation of bulk and boundary effects

Now we compute the Gaussian S-matrix. In Sec. 3.1, we obtain the S-matrix in the leading saddle-point approximation (18) for the large widths expansion. In Sec. 3.2, we exactly integrate over the spacetime position x of the interaction point. In Sec. 3.3, we separate the bulk and boundary effects. In Sec. 3.4, a limit of large argument is taken to get some physical insight. A schematic figure for this section is presented in Fig. 1.

3.1. Saddle-point approximation in plane-wave limit

With the leading saddle-point approximation of Eq. (18) in the large-width expansion for all the in and out wave packets, we obtain the S-matrix for a given configuration (Π_0, Π_1, Π_2):[11]

$$S \to \frac{i\kappa}{\sqrt{2}} \left(\prod_{A=0}^{2} (\pi \sigma_A)^{-3/4} \frac{1}{\sqrt{2E_A}} \right) e^{-\frac{\sigma_t}{2}(\delta\omega)^2 - \frac{\sigma_s}{2}(\delta \boldsymbol{P})^2 - \frac{\mathcal{R}}{2} + i[\cdots]}$$
$$\times \int_{T_\text{in}}^{T_\text{out}} dt\, e^{-\frac{1}{2\sigma_t}[t-(\mathfrak{T}+i\sigma_t\delta\omega)]^2} \int d^3\boldsymbol{x}\, e^{-\frac{1}{2\sigma_s}\left[\boldsymbol{x}-\left(\overline{\boldsymbol{\mathfrak{X}}}+\overline{\boldsymbol{V}}t-i\sigma_s\delta\boldsymbol{P}\right)\right]^2}, \tag{27}$$

where the symbols indicate the following:

- E_A are the on-shell energies:

$$E_A := \sqrt{m_A^2 + \boldsymbol{P}_A^2} \qquad (A = 0, 1, 2), \tag{28}$$

  with $m_0 := m_\Phi$ and $m_a := m_\phi$ $(a = 1, 2)$ being their masses—this is merely a rephrasing of Eq. (3).
- $\boldsymbol{V}_A$ are the corresponding group velocities:

$$\boldsymbol{V}_A := \frac{\boldsymbol{P}_A}{E_A}. \tag{29}$$

  We may freely choose either variable $\boldsymbol{P}_A$ or $\boldsymbol{V}_A$, which are in one-to-one correspondence.
- $\sqrt{\sigma_s}$ is the spatial size of the interaction region:

$$\sigma_s := \left(\sum_{A=0}^{2} \frac{1}{\sigma_A} \right)^{-1}. \tag{30}$$

  Hereafter, we abbreviate e.g. $\sum_{A=0}^{2}$ to $\sum_A$. (We also let the lower-case letters $a, b, \ldots$ run for the final states 1 and 2 such that $\sum_a := \sum_{a=1}^{2}$, etc.)
- The overline denotes the following weighted sum (and not the complex conjugate): For arbitrary scalar and three-vector quantities C_A and $\boldsymbol{Q}_A$, respectively, we define

$$\overline{C} := \sigma_s \sum_A \frac{C_A}{\sigma_A}, \qquad \overline{\boldsymbol{Q}} := \sigma_s \sum_A \frac{\boldsymbol{Q}_A}{\sigma_A}. \tag{31}$$

  We further define, for any $\boldsymbol{Q}_A$,

$$\Delta \boldsymbol{Q}^2 := \overline{\boldsymbol{Q}^2} - \overline{\boldsymbol{Q}}^2, \tag{32}$$

  where $\overline{\boldsymbol{Q}^2} = \sigma_s \sum_A \frac{\boldsymbol{Q}_A^2}{\sigma_A}$ and $\overline{\boldsymbol{Q}}^2 = \overline{\boldsymbol{Q}} \cdot \overline{\boldsymbol{Q}} = \sigma_s^2 \sum_{AB} \frac{\boldsymbol{Q}_A \cdot \boldsymbol{Q}_B}{\sigma_A \sigma_B}$, which follow from the definition in Eq. (31).
- $\sqrt{\sigma_t}$ is the time-like size of the interaction region:

$$\sigma_t := \frac{\sigma_s}{\Delta \boldsymbol{V}^2}. \tag{33}$$

[11] Recall that we abbreviate $(\sigma_0, \Pi_0; \sigma_1, \Pi_1; \sigma_2, \Pi_2)$ to (Π_0, Π_1, Π_2).

- $\mathfrak{T}$ is what we call the *intersection time*, around which the interaction occurs:

$$\mathfrak{T} := \sigma_t \frac{\overline{\boldsymbol{V}} \cdot \overline{\boldsymbol{\mathfrak{X}}} - \overline{\boldsymbol{V} \cdot \boldsymbol{\mathfrak{X}}}}{\sigma_s} = \frac{\overline{\boldsymbol{V}} \cdot \overline{\boldsymbol{\mathfrak{X}}} - \overline{\boldsymbol{V} \cdot \boldsymbol{\mathfrak{X}}}}{\Delta \boldsymbol{V}^2}, \tag{34}$$

  where $\boldsymbol{\mathfrak{X}}_A = \boldsymbol{\Xi}_A(0)$ is the location of the center of each wave packet at our reference time $t = 0$:

$$\boldsymbol{\mathfrak{X}}_A := \boldsymbol{X}_A - \boldsymbol{V}_A T_A. \tag{35}$$

- $\mathcal{R}$ is what we will call the *overlap exponent* that gives the suppression factor accounting for the non-overlap of the wave packets at the intersection point:

$$\mathcal{R} := \frac{\Delta \boldsymbol{\mathfrak{X}}^2}{\sigma_s} - \frac{\mathfrak{T}^2}{\sigma_t}. \tag{36}$$

- We define the momentum and energy shifts, etc., as:

$$\delta \boldsymbol{P} := \boldsymbol{P}_1 + \boldsymbol{P}_2 - \boldsymbol{P}_0, \qquad \delta E := E_1 + E_2 - E_0, \qquad \delta\omega := \delta E - \overline{\boldsymbol{V}} \cdot \delta \boldsymbol{P}. \tag{37}$$

- "$i\,[\cdots]$" denotes the irrelevant pure imaginary terms that are independent of x. We will neglect them hereafter as they disappear when we take the absolute square of S.

Note that each quantity defined in the above list is a fixed real number for a given configuration of the wave packets (Π_0, Π_1, Π_2). Later we will treat $\boldsymbol{X}_a$ $(a = 1, 2)$ as variables of six degrees of freedom; $\mathfrak{T}$, $\boldsymbol{\mathfrak{X}}_a$, and $\mathcal{R}$ are dependent ones. (If we vary the final state momenta then $\boldsymbol{P}_a$ $(a = 1, 2)$ also become variables; $\boldsymbol{V}_a$, σ_t, $\delta \boldsymbol{P}$, δE, and $\delta\omega$ become dependent ones accordingly.)

For any pair of three-vectors $\boldsymbol{Q}_A$ and $\boldsymbol{Q}'_A$ $(A = 0, 1, 2)$, we get

$$\overline{\boldsymbol{Q} \cdot \boldsymbol{Q}'} - \overline{\boldsymbol{Q}} \cdot \overline{\boldsymbol{Q}'} = \sigma_s^2 \left[\frac{\delta \boldsymbol{Q}_1 \cdot \delta \boldsymbol{Q}'_1}{\sigma_0 \sigma_1} + \frac{\delta \boldsymbol{Q}_2 \cdot \delta \boldsymbol{Q}'_2}{\sigma_0 \sigma_2} + \frac{(\delta \boldsymbol{Q}_1 - \delta \boldsymbol{Q}_2) \cdot (\delta \boldsymbol{Q}'_1 - \delta \boldsymbol{Q}'_2)}{\sigma_1 \sigma_2} \right], \tag{38}$$

where we define, for any $\boldsymbol{Q}_A$,[12]

$$\delta \boldsymbol{Q}_a := \boldsymbol{Q}_a - \boldsymbol{Q}_0. \tag{39}$$

Note that we always have $\delta \boldsymbol{Q}_1 - \delta \boldsymbol{Q}_2 = \boldsymbol{Q}_1 - \boldsymbol{Q}_2$. In particular,

$$\begin{aligned} \Delta \boldsymbol{Q}^2 &= \sigma_s^2 \left[\frac{(\delta \boldsymbol{Q}_1)^2}{\sigma_0 \sigma_1} + \frac{(\delta \boldsymbol{Q}_2)^2}{\sigma_0 \sigma_2} + \frac{(\delta \boldsymbol{Q}_1 - \delta \boldsymbol{Q}_2)^2}{\sigma_1 \sigma_2} \right] \\ &= \sigma_s^2 \left[\frac{(\boldsymbol{Q}_1 - \boldsymbol{Q}_0)^2}{\sigma_0 \sigma_1} + \frac{(\boldsymbol{Q}_2 - \boldsymbol{Q}_0)^2}{\sigma_0 \sigma_2} + \frac{(\boldsymbol{Q}_1 - \boldsymbol{Q}_2)^2}{\sigma_1 \sigma_2} \right], \end{aligned} \tag{40}$$

or more concretely,

$$\Delta \boldsymbol{\mathfrak{X}}^2 = \sigma_s^2 \left[\frac{(\delta \boldsymbol{\mathfrak{X}}_1)^2}{\sigma_0 \sigma_1} + \frac{(\delta \boldsymbol{\mathfrak{X}}_2)^2}{\sigma_0 \sigma_2} + \frac{(\delta \boldsymbol{\mathfrak{X}}_1 - \delta \boldsymbol{\mathfrak{X}}_2)^2}{\sigma_1 \sigma_2} \right], \tag{41}$$

[12] The abuse of notation for δ in Eq. (37) should be understood.

$$\Delta \boldsymbol{V}^2 = \sigma_s^2 \left[\frac{(\delta \boldsymbol{V}_1)^2}{\sigma_0\sigma_1} + \frac{(\delta \boldsymbol{V}_2)^2}{\sigma_0\sigma_2} + \frac{(\delta \boldsymbol{V}_1 - \delta \boldsymbol{V}_2)^2}{\sigma_1\sigma_2} \right]. \tag{42}$$

Then we get

$$\sigma_t = \frac{1}{\sigma_s} \left[\frac{(\delta \boldsymbol{V}_1)^2}{\sigma_0\sigma_1} + \frac{(\delta \boldsymbol{V}_2)^2}{\sigma_0\sigma_2} + \frac{(\delta \boldsymbol{V}_1 - \delta \boldsymbol{V}_2)^2}{\sigma_1\sigma_2} \right]^{-1}, \tag{43}$$

$$\mathfrak{T} = -\sigma_s\sigma_t \left[\frac{\delta \boldsymbol{\mathfrak{X}}_1 \cdot \delta \boldsymbol{V}_1}{\sigma_0\sigma_1} + \frac{\delta \boldsymbol{\mathfrak{X}}_2 \cdot \delta \boldsymbol{V}_2}{\sigma_0\sigma_2} + \frac{(\delta \boldsymbol{\mathfrak{X}}_1 - \delta \boldsymbol{\mathfrak{X}}_2) \cdot (\delta \boldsymbol{V}_1 - \delta \boldsymbol{V}_2)}{\sigma_1\sigma_2} \right], \tag{44}$$

$$\begin{aligned} \mathcal{R} = \sigma_s \Bigg\{ & \frac{(\delta \boldsymbol{\mathfrak{X}}_1)^2}{\sigma_0\sigma_1} + \frac{(\delta \boldsymbol{\mathfrak{X}}_2)^2}{\sigma_0\sigma_2} + \frac{(\delta \boldsymbol{\mathfrak{X}}_1 - \delta \boldsymbol{\mathfrak{X}}_2)^2}{\sigma_1\sigma_2} \\ & - \sigma_s\sigma_t \left[\frac{\delta \boldsymbol{\mathfrak{X}}_1 \cdot \delta \boldsymbol{V}_1}{\sigma_0\sigma_1} + \frac{\delta \boldsymbol{\mathfrak{X}}_2 \cdot \delta \boldsymbol{V}_2}{\sigma_0\sigma_2} + \frac{(\delta \boldsymbol{\mathfrak{X}}_1 - \delta \boldsymbol{\mathfrak{X}}_2) \cdot (\delta \boldsymbol{V}_1 - \delta \boldsymbol{V}_2)}{\sigma_1\sigma_2} \right]^2 \Bigg\}. \end{aligned} \tag{45}$$

Note that for a parent particle at rest, $\boldsymbol{P}_0 = 0$, we may simply replace $\delta \boldsymbol{V}_a \to \boldsymbol{V}_a$. Expressions in various limits are shown in Appendix C.

Let us prove the non-negativity of $\mathcal{R}$. In general, the weighted average for any real vector $\boldsymbol{Q}$ satisfies

$$\Delta \boldsymbol{Q}^2 = \overline{\boldsymbol{Q}^2} - \overline{\boldsymbol{Q}}^2 = \overline{\left(\boldsymbol{Q} - \overline{\boldsymbol{Q}}\right)^2} \geq 0. \tag{46}$$

From this, one can deduce the non-negativity of $\mathcal{R}$ as follows: At time t, the center of each wave packet is located at

$$\boldsymbol{Z}_A := \boldsymbol{\mathfrak{X}}_A + \boldsymbol{V}_A t. \tag{47}$$

The square completion of $\Delta \boldsymbol{Z}^2 = \overline{\boldsymbol{Z}^2} - \overline{\boldsymbol{Z}}^2$ with respect to t shows that $\Delta \boldsymbol{Z}^2$ takes its minimum value $\sigma_s \mathcal{R}$ at $t = \mathfrak{T}$:

$$\Delta \boldsymbol{Z}^2 = \Delta \boldsymbol{V}^2 \left(t - \mathfrak{T}\right)^2 + \sigma_s \mathcal{R}. \tag{48}$$

As $\Delta \boldsymbol{Z}^2 \geq 0$ for any t, we obtain $\sigma_s \mathcal{R} \geq 0$, hence the non-negativity of $\mathcal{R}$.

In particular, if the center of all three wave packets coincide at $\boldsymbol{Z}_A = \boldsymbol{x}$ at some time t, then $\overline{\boldsymbol{Z}} = \boldsymbol{x}$ and $\Delta \boldsymbol{Z}^2 = 0$. Equation (48) shows that this can be the case when and only when $t = \mathfrak{T}$ (for $\Delta \boldsymbol{V}^2 > 0$), and that we get no suppression in such a case, $\mathcal{R} = 0$.

Let us see the physical meaning of $\mathfrak{T}$. Suppose that we recklessly take the particle limit $\sigma_t, \sigma_s \to 0$ in the second line in Eq. (27) even though the expression itself is obtained in the contrary plane-wave expansion. Then we see that the interaction indeed occurs around the spacetime point

$$x = (t, \boldsymbol{x}) \sim \left(\mathfrak{T}, \overline{\boldsymbol{\mathfrak{X}}} + \overline{\boldsymbol{V}}\mathfrak{T}\right), \tag{49}$$

which we call the *intersection point*.

One can show (without taking the particle limit) that the intersection point in Eq. (49) is transformed properly by spacetime translation: By a constant spacetime translation

$$\begin{aligned} \boldsymbol{X}_A &\to \boldsymbol{X}_A + \boldsymbol{d}, \\ T_A &\to T_A + d^0, \end{aligned} \tag{50}$$

the center of each wave packet (at $t = 0$) and its average transform as

$$\boldsymbol{\mathfrak{X}}_A \to \boldsymbol{\mathfrak{X}}_A + \boldsymbol{d} - \boldsymbol{V}_A d^0, \tag{51}$$

$$\overline{\boldsymbol{\mathfrak{X}}} \to \overline{\boldsymbol{\mathfrak{X}}} + \boldsymbol{d} - \overline{\boldsymbol{V}} d^0, \tag{52}$$

and hence

$$\mathfrak{T} \to \mathfrak{T} + d^0, \tag{53}$$

$$\left(\overline{\boldsymbol{\mathfrak{X}}} + \overline{\boldsymbol{V}}\mathfrak{T}\right) \to \left(\overline{\boldsymbol{\mathfrak{X}}} + \overline{\boldsymbol{V}}\mathfrak{T}\right) + \boldsymbol{d}. \tag{54}$$

One can also check that the overlap exponent $\mathcal{R}$ is translationally invariant (as it should physically be):

$$\mathcal{R} \to \mathcal{R}. \tag{55}$$

In particular, we may choose

$$\boldsymbol{d} = \boldsymbol{V}_0 d^0, \tag{56}$$

such that the center of the initial wave packet at $t = 0$, $\boldsymbol{\mathfrak{X}}_0 = \boldsymbol{X}_0 - \boldsymbol{V}_0 T_0$, is kept invariant. Then the center of each final-state wave packet, $\boldsymbol{\mathfrak{X}}_a$, is shifted as[13]

$$\boldsymbol{\mathfrak{X}}_a \to \boldsymbol{\mathfrak{X}}_a - \delta\boldsymbol{V}_a d^0, \qquad \delta\boldsymbol{\mathfrak{X}}_a \to \delta\boldsymbol{\mathfrak{X}}_a - \delta\boldsymbol{V}_a d^0. \tag{57}$$

Later, this translation will correspond to the zero mode, Eq. (91).

3.2. *Spacetime integral over the position of the interaction point*

One can exactly perform the Gaussian integrals over the interaction point $x = (t, \boldsymbol{x})$ in Eq. (27) to get

$$S = \frac{i\kappa}{\sqrt{2}} \left(\prod_A (\pi\sigma_A)^{-3/4} \frac{1}{\sqrt{2E_A}} \right) e^{-\frac{\sigma_t}{2}(\delta\omega)^2 - \frac{\sigma_s}{2}(\delta\boldsymbol{P})^2 - \frac{\mathcal{R}}{2}} (2\pi\sigma_s)^{3/2} \sqrt{2\pi\sigma_t}\, G(\mathfrak{T}), \tag{58}$$

where we have defined the *window function*,

$$\begin{aligned} G(\mathfrak{T}) &:= \int_{T_\text{in}}^{T_\text{out}} \frac{dt}{\sqrt{2\pi\sigma_t}} e^{-\frac{1}{2\sigma_t}(t - \mathfrak{T} - i\sigma_t\delta\omega)^2} \\ &= \frac{1}{2}\left[\operatorname{erf}\left(\frac{\mathfrak{T} - T_\text{in} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right) - \operatorname{erf}\left(\frac{\mathfrak{T} - T_\text{out} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)\right], \end{aligned} \tag{59}$$

in which

$$\operatorname{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z e^{-x^2} dx \tag{60}$$

is the Gauss error function. In the small- and large-$|z|$ limits, its (asymptotic) expansion reads, respectively,

$$\operatorname{erf}(z) = \frac{2z}{\sqrt{\pi}} + \mathcal{O}\left(z^3\right), \tag{61}$$

[13] The average over the initial and final states is shifted as $\overline{\boldsymbol{\mathfrak{X}}} \to \overline{\boldsymbol{\mathfrak{X}}} - \left(\overline{\boldsymbol{V}} - \boldsymbol{V}_0\right) d^0$.

$$\operatorname{erf}(z) = \operatorname{sgn}(z) + e^{-z^2}\left(-\frac{1}{\sqrt{\pi}z} + \mathcal{O}\left(z^{-3}\right)\right), \tag{62}$$

where we have defined a sign function for a complex variable:

$$\operatorname{sgn}(z) := \begin{cases} 1 & \text{for } \Re z > 0 \text{ or } (\Re z = 0 \text{ and } \Im z > 0), \\ -1 & \text{for } \Re z < 0 \text{ or } (\Re z = 0 \text{ and } \Im z < 0), \\ 0 & \text{for } z = 0. \end{cases} \tag{63}$$

From Eq. (58), we see that the S-matrix is exponentially suppressed unless the momentum is nearly conserved, $\delta \boldsymbol{P} \sim 0$. This is also the case for the energy conservation $\delta\omega \sim 0$ except in the boundary regions, at which the translational invariance is explicitly broken; see Sect. 3.4 below. As stated above, the overlap exponent $\mathcal{R}$ gives another suppression when the wave packets do not overlap.

3.3. *Separation of bulk and boundary effects*

It is convenient to separate the window function in Eq. (59) into the bulk part and the in- and out-boundary ones:

$$G(\mathfrak{T}) = G_{\text{bulk}}(\mathfrak{T}) + G_{\text{in-bdry}}(\mathfrak{T}) + G_{\text{out-bdry}}(\mathfrak{T}), \tag{64}$$

where

$$G_{\text{bulk}}(\mathfrak{T}) := \frac{1}{2}\left[\operatorname{sgn}\left(\frac{\mathfrak{T} - T_{\text{in}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right) - \operatorname{sgn}\left(\frac{\mathfrak{T} - T_{\text{out}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)\right], \tag{65}$$

$$G_{\text{in-bdry}}(\mathfrak{T}) := \frac{1}{2}\left[\operatorname{erf}\left(\frac{\mathfrak{T} - T_{\text{in}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right) - \operatorname{sgn}\left(\frac{\mathfrak{T} - T_{\text{in}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)\right],$$

$$G_{\text{out-bdry}}(\mathfrak{T}) := \frac{1}{2}\left[\operatorname{sgn}\left(\frac{\mathfrak{T} - T_{\text{out}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right) - \operatorname{erf}\left(\frac{\mathfrak{T} - T_{\text{out}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)\right]. \tag{66}$$

One can rewrite the boundary parts:

$$G_{\text{in-bdry}}(\mathfrak{T}) = \frac{1}{2}G_{\text{bdry}}\left(\frac{\mathfrak{T} - T_{\text{in}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right), \tag{67}$$

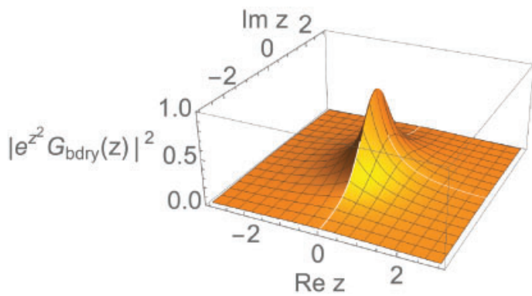
$$G_{\text{out-bdry}}(\mathfrak{T}) = -\frac{1}{2}G_{\text{bdry}}\left(\frac{\mathfrak{T} - T_{\text{out}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right), \tag{68}$$

where

$$G_{\text{bdry}}(z) := \operatorname{erf}(z) - \operatorname{sgn}(z). \tag{69}$$

More explicitly, the bulk part reads

$$G_{\text{bulk}}(\mathfrak{T}) = \begin{cases} 1 & (T_{\text{in}} < \mathfrak{T} < T_{\text{out}}), \\ 0 & (\mathfrak{T} < T_{\text{in}} \text{ or } T_{\text{out}} < \mathfrak{T}), \\ \theta(\delta\omega) & (\mathfrak{T} = T_{\text{in}}), \\ \theta(-\delta\omega) & (\mathfrak{T} = T_{\text{out}}), \end{cases} \tag{70}$$



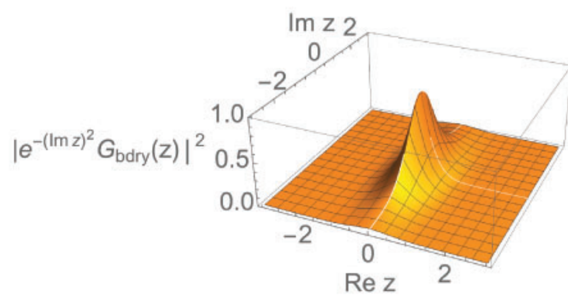


Fig. 2. Normalized boundary function $\left|e^{z^2}G_{\text{bdry}}(z)\right|^2$ (left) and the combination that appears in the physical setup $\left|e^{-(\Im z)^2}G_{\text{bdry}}(z)\right|^2$ (right).

where

$$\theta(x) = \frac{1+\text{sgn}(x)}{2} = \begin{cases} 1 & (x>0), \\ \frac{1}{2} & (x=0), \\ 0 & (x<0), \end{cases} \tag{71}$$

is the step function.[14]

We note that $G_{\text{bdry}}(z)$ is discontinuous at $\Re z = 0$ but the combination $\left|e^{z^2}G_{\text{bdry}}(z)\right|^2$ is continuous and finite everywhere on the complex z plane (except at the origin $z=0$); see Fig. 2. In particular, in the limit $|z| \to \infty$, we obtain[15]

$$\left|e^{z^2}G_{\text{bdry}}(z)\right|^2 \to \frac{1}{\pi\,|z|^2}. \tag{72}$$

The explicit formula in the boundary limit $|\mathfrak{T} - T_{\text{in/out}}| \ll \sigma_t\delta\omega$ is

$$G_{\text{bdry}}\left(\frac{\mathfrak{T} - T_{\text{in/out}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right) \to \pm\frac{2i}{\sqrt{\pi}}F\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right)e^{\frac{\sigma_t}{2}(\delta\omega)^2} \mp \begin{cases} \text{sgn}(\delta\omega) & \text{for } \mathfrak{T} = T_{\text{in/out}}, \\ \text{sgn}(\mathfrak{T} - T_{\text{in/out}}) & \text{for } \mathfrak{T} \neq T_{\text{in/out}}, \end{cases} \tag{73}$$

that is,[16]

$$e^{-\sigma_t(\delta\omega)^2}\left|G_{\text{bdry}}\left(\frac{\mathfrak{T} - T_{\text{in/out}} + i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)\right|^2 \to \frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right) + e^{-\sigma_t(\delta\omega)^2}, \tag{74}$$

where

$$F(x) := e^{-x^2}\int_0^x e^{z^2}dz = -i\frac{\sqrt{\pi}}{2}e^{-x^2}\,\text{erf}\,(ix) \tag{75}$$

[14] As we see in Eq. (70), this step function appears only at $\mathfrak{T} = T_{\text{in/out}}$ and hence does not contribute when summed with G_{bdry} and integrated over $\mathfrak{T}$. That is, it appears only at $\Re z = 0$ and does not contribute when integrated over $\Re z$ in Fig. 2. This might be non-vanishing for a more realistic non-Gaussian wave packet.

[15] In terms of the relevant combination, we get

$$e^{-2(\Im z)^2}\left|G_{\text{bdry}}(z)\right|^2 \to \frac{e^{-2(\Re z)^2}}{\pi\,|z|^2}.$$

[16] We have assumed $\mathfrak{T} - T_{\text{in/out}} + i\sigma_t\delta\omega \neq 0$ in writing $\text{sgn}^2 = 1$.

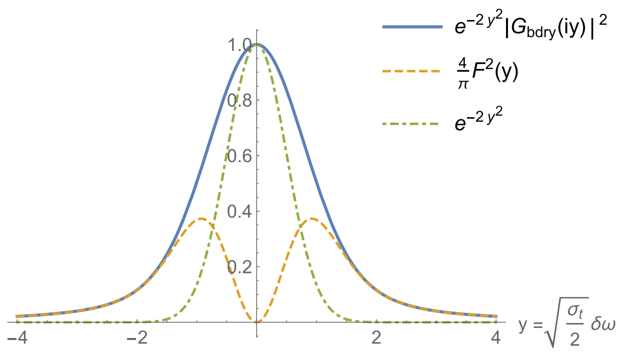


Fig. 3. $e^{-2y^2}\left|G_{\text{bdry}}(iy)\right|^2$ (solid), $\frac{4}{\pi}F^2(y)$ (dashed), and e^{-2y^2} (dot-dashed) as a function of $y=\sqrt{\frac{\sigma_t}{2}}\delta\omega$, which corresponds to right on either boundary $\mathfrak{T}=T_{\text{in/out}}$. The solid line is the sum of the dashed and dot-dashed lines and corresponds to the ridge line at $\Re z=0$ in Fig. 2.

is the Dawson function, whose (asymptotic) expansions read

$$F(x)=x+\mathcal{O}\left(x^3\right), \tag{76}$$

$$F(x)=-i\frac{\sqrt{\pi}}{2}e^{-x^2}\operatorname{sgn}(ix)+\frac{1}{2x}+\mathcal{O}\left(\frac{1}{x^3}\right). \tag{77}$$

More explicitly, the large-$\sqrt{\sigma_t}\delta\omega$ expansion gives

$$\frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right)+e^{-\sigma_t(\delta\omega)^2}=\frac{2}{\pi}\frac{1}{\sigma_t\,(\delta\omega)^2}+\mathcal{O}\left(\frac{1}{\sigma_t^2\,(\delta\omega)^4}\right). \tag{78}$$

In Fig. 3, we plot G_{bdry} right at either boundary $\mathfrak{T}=T_{\text{in/out}}$.

3.4. *Limit of large argument*

In the limit

$$\frac{|\mathfrak{T}-T_{\text{in}}+i\sigma_t\delta\omega|}{\sqrt{\sigma_t}},\frac{|\mathfrak{T}-T_{\text{out}}+i\sigma_t\delta\omega|}{\sqrt{\sigma_t}}\gg 1, \tag{79}$$

the possible leading contributions are

$$\begin{aligned}G(\mathfrak{T})\to{}&\frac{1}{2}\left[\operatorname{sgn}\left(\frac{\mathfrak{T}-T_{\text{in}}+i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)-\operatorname{sgn}\left(\frac{\mathfrak{T}-T_{\text{out}}+i\sigma_t\delta\omega}{\sqrt{2\sigma_t}}\right)\right]\\&-e^{-\frac{(\mathfrak{T}-T_{\text{in}})^2}{2\sigma_t}+\frac{\sigma_t}{2}(\delta\omega)^2-i\,\delta\omega(\mathfrak{T}-T_{\text{in}})}\sqrt{\frac{2\sigma_t}{\pi}}\frac{1}{\mathfrak{T}-T_{\text{in}}+i\sigma_t\delta\omega}\\&+e^{-\frac{(\mathfrak{T}-T_{\text{out}})^2}{2\sigma_t}+\frac{\sigma_t}{2}(\delta\omega)^2-i\,\delta\omega(\mathfrak{T}-T_{\text{out}})}\sqrt{\frac{2\sigma_t}{\pi}}\frac{1}{\mathfrak{T}-T_{\text{out}}+i\sigma_t\delta\omega}.\end{aligned} \tag{80}$$

We see that the range of $\mathfrak{T}$ in this limit can be separated into the following regions:

- In the *bulk region*

$$|\mathfrak{T}-T_{\text{in}}|\,,|\mathfrak{T}-T_{\text{out}}|\gg\sigma_t\delta\omega, \tag{81}$$

where the intersection time $\mathfrak{T}$ is well separated from both the boundary times T_{in} and T_{out}, we obtain

$$G(\mathfrak{T}) \to W(\mathfrak{T}) := \begin{cases} 1 & (T_{\text{in}} < \mathfrak{T} < T_{\text{out}}), \\ 0 & (\text{otherwise}), \end{cases} \tag{82}$$

hence the name "window function."

- In the *in* and *out boundary regions* $\mathfrak{T} \sim T_{\text{in}}$ and T_{out} (namely $|\mathfrak{T} - T_{\text{in}}| \lesssim \sigma_t \delta\omega$ and $|\mathfrak{T} - T_{\text{out}}| \lesssim \sigma_t \delta\omega$), the contribution from the second and third lines, respectively, in Eq. (80) becomes sizable:

$$e^{-\sigma_t(\delta\omega)^2} |G(\mathfrak{T})|^2 \to e^{-\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t}} \frac{2}{\pi} \frac{1}{\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t} + \sigma_t (\delta\omega)^2}. \tag{83}$$

We see that the exponential suppression $e^{-\sigma_t(\delta\omega)^2}$ for $\sigma_t (\delta\omega)^2 \gg 1$ becomes absent in the boundary region.

In Refs. [8–11], the authors have claimed that contributions from the boundary region can become non-negligible and that there can be physical consequences.[17] In this paper we leave this issue open and proceed by taking into account only the bulk region contribution of Eq. (82); we will briefly comment on the boundary effects in Sect. 4.3.

Equation (83) appears singular in the simultaneous limit $|\mathfrak{T} - T_{\text{in/out}}| \to 0$ and $\sigma_t \delta\omega \to 0$. This apparent singularity is an artifact of first taking the limit in Eq. (80): If we take the limit $|\mathfrak{T} - T_{\text{in/out}} + i\sigma_t\delta\omega| \ll \sqrt{\sigma_t}$ in the original expression, Eq. (59), we obtain

$$e^{-\sigma_t(\delta\omega)^2} |G(\mathfrak{T})|^2 \to \frac{(\mathfrak{T} - T_{\text{in/out}})^2 + (\sigma_t \delta\omega)^2}{2\pi\sigma_t}. \tag{84}$$

It is manifest that we have no singularity.

4. Decay probability: derivation of Fermi's golden rule

Recalling the (over-)completeness of the Gaussian basis in Eq. (A.22), we see that the decay probability into an infinitesimal phase-space range $[\boldsymbol{X}_a, \boldsymbol{X}_a + d\boldsymbol{X}_a]$ and $[\boldsymbol{P}_a, \boldsymbol{P}_a + d\boldsymbol{P}_a]$ $(a = 1, 2)$ is

$$\begin{aligned} dP &= \frac{d^3\boldsymbol{X}_1\, d^3\boldsymbol{P}_1}{(2\pi)^3} \frac{d^3\boldsymbol{X}_2\, d^3\boldsymbol{P}_2}{(2\pi)^3} |S|^2 \\ &= \frac{\kappa^2}{2} \frac{1}{2E_0} \frac{d^3\boldsymbol{P}_1}{(2\pi)^3\, 2E_1} \frac{d^3\boldsymbol{P}_2}{(2\pi)^3\, 2E_2} (2\pi)^4 \left(\sqrt{\frac{\sigma_t}{\pi}} e^{-\sigma_t(\delta\omega)^2} \right) \left(\left(\frac{\sigma_s}{\pi}\right)^{3/2} e^{-\sigma_s(\delta\boldsymbol{P})^2} \right) \\ &\quad \times \sqrt{\frac{\sigma_t}{\pi^5} \left(\frac{\sigma_s}{\sigma_0\sigma_1\sigma_2} \right)^3} d^3\boldsymbol{X}_1\, d^3\boldsymbol{X}_2\, e^{-\mathcal{R}}\, |G(\mathfrak{T})|^2 . \end{aligned} \tag{85}$$

[17] One might need a justification for placing the interaction around $T_{\text{in/out}}$, which are defined to be the times at which the very interactions are negligible; see Eq. (22). Note that this contradiction in identifying the in-state with the free state at the remote past, as in Eq. (9), already exists in the ordinary plane-wave computation of the *decay* rate because the interaction for the decay never becomes negligible even in the infinite-past limit, and one needs to dump the interaction by hand by introducing the $\pm i\epsilon$ term. A better treatment would be to take into account the production process of the parent particle, namely, to compute the $\phi\phi \to \phi\phi$ scattering and the one-loop correction to it in the wave-packet formalism, which will be presented elsewhere.

We note that this expression is exact up to the leading saddle-point approximation, Eq. (18).

In Sect. 4.1 we show how to diagonalize the overlap exponent $\mathcal{R}$. In Sect. 4.2 we focus on the bulk contribution G_{bulk} and derive Fermi's golden rule. In Sect. 4.3, we briefly comment on the boundary contribution G_{bdry}.

4.1. Diagonalization of the overlap exponent

Now we want to perform the Gaussian integral over the central positions of the wave packets $\boldsymbol{X}_a$. We may rewrite $\mathcal{R}$, in matrix notation, as follows:

$$\mathcal{R} = \begin{bmatrix} \delta\mathfrak{X}_1^{\text{t}} & \delta\mathfrak{X}_2^{\text{t}} \end{bmatrix} \mathcal{M} \begin{bmatrix} \delta\mathfrak{X}_1 \\ \delta\mathfrak{X}_2 \end{bmatrix}, \tag{86}$$

where the superscript "t" denotes transposition; as defined in Eq. (39),

$$\delta\mathfrak{X}_a := \mathfrak{X}_a - \mathfrak{X}_0, \qquad \delta\boldsymbol{V}_a := \boldsymbol{V}_a - \boldsymbol{V}_0, \tag{87}$$

for $a = 1, 2$; and $\mathcal{M}$ is the following real symmetric 6×6 matrix:

$$\mathcal{M} = \frac{\sigma_s}{\sigma_1\sigma_2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{\sigma_s}{\sigma_0}\begin{bmatrix} \frac{1}{\sigma_1} & 0 \\ 0 & \frac{1}{\sigma_2} \end{bmatrix} + \sigma_s^2\sigma_t \begin{bmatrix} \widetilde{\delta\boldsymbol{V}}_1 \widetilde{\delta\boldsymbol{V}}_1^{\text{t}} & \widetilde{\delta\boldsymbol{V}}_1 \widetilde{\delta\boldsymbol{V}}_2^{\text{t}} \\ \widetilde{\delta\boldsymbol{V}}_2 \widetilde{\delta\boldsymbol{V}}_1^{\text{t}} & \widetilde{\delta\boldsymbol{V}}_2 \widetilde{\delta\boldsymbol{V}}_2^{\text{t}} \end{bmatrix}, \tag{88}$$

in which

$$\widetilde{\delta\boldsymbol{V}}_1 := \frac{\delta\boldsymbol{V}_1}{\sigma_0\sigma_1} + \frac{\delta\boldsymbol{V}_1 - \delta\boldsymbol{V}_2}{\sigma_1\sigma_2} = \frac{1}{\sigma_1}\left[\left(\frac{1}{\sigma_0} + \frac{1}{\sigma_2}\right)\delta\boldsymbol{V}_1 - \frac{\delta\boldsymbol{V}_2}{\sigma_2}\right], \tag{89}$$

$$\widetilde{\delta\boldsymbol{V}}_2 := \frac{\delta\boldsymbol{V}_2}{\sigma_0\sigma_2} - \frac{\delta\boldsymbol{V}_1 - \delta\boldsymbol{V}_2}{\sigma_1\sigma_2} = \frac{1}{\sigma_2}\left[\left(\frac{1}{\sigma_0} + \frac{1}{\sigma_1}\right)\delta\boldsymbol{V}_2 - \frac{\delta\boldsymbol{V}_1}{\sigma_1}\right]. \tag{90}$$

Hereafter, we employ the shifted $\delta\mathfrak{X}_a = \boldsymbol{X}_a - (\boldsymbol{V}_a T_a + \boldsymbol{X}_0 - \boldsymbol{V}_0 T_0)$ as six integration variables.

One can check that $\mathcal{M}$ has a zero eigenvector:

$$\mathcal{M}\vec{\mathcal{X}}_0 = 0, \qquad \vec{\mathcal{X}}_0 = \frac{1}{\sqrt{(\delta\boldsymbol{V}_1)^2 + (\delta\boldsymbol{V}_2)^2}}\begin{bmatrix} \delta\boldsymbol{V}_1 \\ \delta\boldsymbol{V}_2 \end{bmatrix}, \tag{91}$$

where we have normalized $\vec{\mathcal{X}}_0$ as $\vec{\mathcal{X}}_0^{\text{t}}\vec{\mathcal{X}}_0 = 1$. This is a direct consequence of the translational invariance under Eq. (57). This zero-mode will eventually give the factor $T_{\text{out}} - T_{\text{in}}$, which is the characteristic of Fermi's golden rule.

Writing the other five normalized eigenvectors as $\vec{\mathcal{X}}_I$ $(I = 1, \ldots, 5)$, we get[18]

$$\mathcal{O}^{\text{t}}\mathcal{M}\mathcal{O} = \text{diag}\,(0, \lambda_1, \ldots, \lambda_5)\,, \qquad \mathcal{M} = \sum_{I=1}^{5} \lambda_I \vec{\mathcal{X}}_I \vec{\mathcal{X}}_I^{\text{t}}, \tag{92}$$

[18] Recall that the zero eigenvector $\vec{\mathcal{X}}_0$ drops out of the spectral representation:

$$\mathcal{M} = \begin{bmatrix} \vec{\mathcal{X}}_0 & \vec{\mathcal{X}}_1 & \cdots & \vec{\mathcal{X}}_5 \end{bmatrix}\begin{bmatrix} 0 & & & \\ & \lambda_1 & & \\ & & \ddots & \\ & & & \lambda_5 \end{bmatrix}\begin{bmatrix} \vec{\mathcal{X}}_0^{\text{t}} \\ \vec{\mathcal{X}}_1^{\text{t}} \\ \vdots \\ \vec{\mathcal{X}}_5^{\text{t}} \end{bmatrix} = \begin{bmatrix} \vec{0} & \vec{\mathcal{X}}_1 & \cdots & \vec{\mathcal{X}}_5 \end{bmatrix}\begin{bmatrix} 0 & & & \\ & \lambda_1 & & \\ & & \ddots & \\ & & & \lambda_5 \end{bmatrix}\begin{bmatrix} \vec{0}^{\text{t}} \\ \vec{\mathcal{X}}_1^{\text{t}} \\ \vdots \\ \vec{\mathcal{X}}_5^{\text{t}} \end{bmatrix}.$$

where $\mathcal{O} := \begin{bmatrix} \vec{\mathcal{X}}_0 & \vec{\mathcal{X}}_1 & \cdots & \vec{\mathcal{X}}_5 \end{bmatrix}$. Explicit forms of the other five eigenvalues $\lambda_1, \dots, \lambda_5$ are

$$\frac{\sigma_s}{2\sigma_0}\left(\frac{1}{\sigma_1}+\frac{1}{\sigma_2}\right)+\frac{\sigma_s}{\sigma_1\sigma_2}\left(1\pm\sqrt{1+\left(\frac{\sigma_1-\sigma_2}{2\sigma_0}\right)^2}\right), \qquad \frac{\sigma_s\sigma_t}{\sigma_0\sigma_1\sigma_2}\left((\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2\right), \tag{93}$$

where we have assumed $\Delta\boldsymbol{V}^2 > 0$ in deriving the former, which is two-fold degenerate per each $\pm$ sign, providing four of the five.[19] After some computation, we obtain

$$\prod_{I=1}^{5}\lambda_I = \sigma_t\left(\frac{\sigma_s}{\sigma_0\sigma_1\sigma_2}\right)^3\left((\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2\right). \tag{94}$$

We define new integration variables $(y_0, y_1, \dots, y_5)$ by

$$\begin{bmatrix} y_0 \\ \vdots \\ y_5 \end{bmatrix} = \mathcal{O}^{\mathrm{t}}\begin{bmatrix} \delta\boldsymbol{\mathfrak{X}}_1 \\ \delta\boldsymbol{\mathfrak{X}}_2 \end{bmatrix}, \qquad \begin{bmatrix} \delta\boldsymbol{\mathfrak{X}}_1 \\ \delta\boldsymbol{\mathfrak{X}}_2 \end{bmatrix} = \mathcal{O}\begin{bmatrix} y_0 \\ \vdots \\ y_5 \end{bmatrix}. \tag{95}$$

In particular, we get

$$y_0 = \frac{\delta\boldsymbol{V}_1\cdot\delta\boldsymbol{\mathfrak{X}}_1+\delta\boldsymbol{V}_2\cdot\delta\boldsymbol{\mathfrak{X}}_2}{\sqrt{(\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2}}. \tag{96}$$

As stated above, the integral over y_0 does not have a Gaussian suppression and will yield the factor $\propto (T_{\mathrm{out}} - T_{\mathrm{in}})$. Note that

$$d^3\boldsymbol{X}_1\, d^3\boldsymbol{X}_2 = d^6y \tag{97}$$

as $\mathcal{O}$ is a special orthogonal matrix.

4.2. Bulk contribution: derivation of Fermi's golden rule

Now we concentrate on the bulk contribution, Eq. (65). Physically, this takes into account the bulk region of Eq. (81), in which the window function takes the particularly simple form of Eq. (82), by which the spatial d^6y integral is confined within the range that satisfies

$$T_{\mathrm{in}} < \mathfrak{T} < T_{\mathrm{out}}, \tag{98}$$

where the explicit form of $\mathfrak{T}$ is given in Eq. (44). We note that $\mathfrak{T}$ is linear in $\delta\boldsymbol{\mathfrak{X}}_a$, and hence in y_I.

In a typical non-singular configuration of $(\boldsymbol{P}_1, \boldsymbol{P}_2)$ with $\Delta\boldsymbol{V}^2 > 0$, the integrals over all the other five variables $y_1, \dots, y_5$ are confined by the Gaussian factor within the range of the order of $\sqrt{\sigma_s}$; see Eq. (93). By definition, the interaction point of the bulk region is well separated from the boundaries,

[19] The eigenvector for the latter is proportional to

$$\begin{bmatrix} \frac{(\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2}{2}\delta\boldsymbol{V}_2-\left((\delta\boldsymbol{V}_1\cdot\delta\boldsymbol{V}_2)-\frac{\sigma_1-\sigma_2}{2\sigma_0}(\delta\boldsymbol{V}_2)^2\right)\delta\boldsymbol{V}_1 \\ \frac{(\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2}{2}\delta\boldsymbol{V}_1-\left((\delta\boldsymbol{V}_1\cdot\delta\boldsymbol{V}_2)+\frac{\sigma_1-\sigma_2}{2\sigma_0}(\delta\boldsymbol{V}_1)^2\right)\delta\boldsymbol{V}_2 \end{bmatrix},$$

which can be explicitly checked to be orthogonal to the zero-eigenvector $\begin{bmatrix} \delta\boldsymbol{V}_1 \\ \delta\boldsymbol{V}_2 \end{bmatrix}$.

and hence the window function can be regarded as unity for the integral over $y_1, \dots, y_5$.[20] That is, we may safely perform each integral over these five variables as simply Gaussian:

$$\int d^5 y\, e^{-\mathcal{R}} = \sqrt{\frac{\pi^5}{\prod_{I=1}^5 \lambda_I}} = \sqrt{\frac{\pi^5}{\sigma_t}\left(\frac{\sigma_0\sigma_1\sigma_2}{\sigma_s}\right)^3} \frac{1}{\sqrt{(\delta \boldsymbol{V}_1)^2 + (\delta \boldsymbol{V}_2)^2}}, \tag{99}$$

in which we used the product of eigenvalues given in Eq. (94).

Rewriting $\delta\boldsymbol{\mathfrak{X}}_a$ in Eq. (44) by $y_0, \dots, y_5$ using the latter of Eq. (95), $\begin{bmatrix}\delta\boldsymbol{\mathfrak{X}}_1\\ \delta\boldsymbol{\mathfrak{X}}_2\end{bmatrix} = \sum_{I=0}^5 \vec{\mathcal{X}}_I\, y_I$, we can read off the coefficient of y_0 in $\mathfrak{T}$. After some computation, we obtain

$$\mathfrak{T} = -\frac{y_0}{\sqrt{(\delta \boldsymbol{V}_1)^2 + (\delta \boldsymbol{V}_2)^2}} + \cdots, \tag{100}$$

where the dots denote the terms linear in $y_1, \dots, y_5$, which are fixed to be of the order of $\sqrt{\sigma_s}$ by the above Gaussian integrals and are neglected hereafter. Now the region of the window function $T_\text{in} < \mathfrak{T} < T_\text{out}$ corresponds to

$$-\sqrt{(\delta \boldsymbol{V}_1)^2 + (\delta \boldsymbol{V}_2)^2}\, T_\text{out} < y_0 < -\sqrt{(\delta \boldsymbol{V}_1)^2 + (\delta \boldsymbol{V}_2)^2}\, T_\text{in}, \tag{101}$$

and the y_0 integral yields

$$\int dy_0 W(\mathfrak{T}) = \sqrt{(\delta \boldsymbol{V}_1)^2 + (\delta \boldsymbol{V}_2)^2}\, (T_\text{out} - T_\text{in}). \tag{102}$$

To summarize, the integral over $(\boldsymbol{X}_1, \boldsymbol{X}_2)$ results in[21]

$$dP = \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\, 2E_1}\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\, 2E_2}(2\pi)^4\left(\sqrt{\frac{\sigma_t}{\pi}}e^{-\sigma_t(\delta\omega)^2}\right)\left(\left(\frac{\sigma_s}{\pi}\right)^{3/2}e^{-\sigma_s(\delta\boldsymbol{P})^2}\right)(T_\text{out} - T_\text{in}). \tag{103}$$

In the wave limit $\sigma_s, \sigma_t \to \infty$, we obtain

$$\frac{dP}{T_\text{out} - T_\text{in}} = \frac{\kappa^2}{2}\frac{1}{2E_0}\left(\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\, 2E_1}\right)\left(\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\, 2E_2}\right)(2\pi)^4\,\delta^4(P_1 + P_2 - P_0). \tag{104}$$

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[20] Though we have taken the leading saddle-point approximation in the large-σ_A expansion in obtaining Eq. (27), we still consider that the wave packets are well localized compared to the whole spacetime volume in which the decay occurs, say $|\mathfrak{T} - T_\text{in/out}| \gg \sqrt{\sigma_s}$. This is consistent with the treatment of the current work restricted within the bulk region.

[21] When the expression for the probability in Eq. (103) grows to the order of unity as one increases $T_\text{out} - T_\text{in}$, one should, e.g., include the phenomenological factor introduced by Weisskopf and Wigner [13,14].

This is nothing but Fermi's golden rule: the decay probability per time interval $T_{\text{out}} - T_{\text{in}}$. The resultant total decay rate reads[22]

$$\frac{P}{T_{\text{out}} - T_{\text{in}}} = \frac{\kappa^2}{32\pi E_0}\sqrt{1 - \frac{4m_\phi^2}{m_\Phi^2}}. \tag{105}$$

4.3. Comments on the boundary contribution

We examine the contributions in Eq. (66), which come from either the in or out boundary region $|\mathfrak{T} - T_{\text{in/out}}| \lesssim \sigma_t \delta\omega$ (tentatively closing our eyes to the point discussed in footnote 17). Formulae for the boundary contributions in the boundary limit are summarized in Appendix D.

Let us estimate the effect of the $d^6 y$ integral over the Gaussian peak $e^{-(\mathfrak{T}-T_{\text{in/out}})^2/\sigma_t}$ in Eq (83), which results from the limit $\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t} + \sigma_t\,(\delta\omega)^2 \gg 1$:

$$dP \to \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\,2E_1}\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\,2E_2}(2\pi)^4\left(\sqrt{\frac{\sigma_t}{\pi}}\right)\left(\left(\frac{\sigma_s}{\pi}\right)^{3/2} e^{-\sigma_s(\delta\boldsymbol{P})^2}\right)$$
$$\times\sqrt{\frac{\sigma_t}{\pi^5}\left(\frac{\sigma_s}{\sigma_0\sigma_1\sigma_2}\right)^3}\, d^6 y\, e^{-\mathcal{R}} e^{-\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t}}\,\frac{2}{\pi}\,\frac{1}{\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t} + \sigma_t\,(\delta\omega)^2}. \tag{106}$$

As discussed in the paragraph containing Eq. (84), this expression is valid only when $\sigma_t\,(\delta\omega)^2 \gg 1$ at $\mathfrak{T} = T_{\text{in/out}}$; see Appendix D for possible generalization.

Naively, the integral over the above-mentioned Gaussian peak would be estimated by taking the formal limit $\sigma_t \to 0$,[23]

$$e^{-\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t}} \to \sqrt{\pi\sigma_t}\,\delta(\mathfrak{T} - T_{\text{in/out}})\,, \tag{107}$$

and by regarding the integral $d^5 y\, e^{-\mathcal{R}}$ as Gaussian, Eq. (99); the remaining y_0 integral would again give the factor $\sqrt{(\delta\boldsymbol{V}_1)^2 + (\delta\boldsymbol{V}_2)^2}$:

$$dP \sim \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\,2E_1}\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\,2E_2}(2\pi)^4\left[\left(\frac{\sigma_s}{\pi}\right)^{3/2} e^{-\sigma_s(\delta\boldsymbol{P})^2}\right]\frac{2}{\pi}\frac{1}{(\delta\omega)^2}. \tag{108}$$

[22] Let us review the textbook computation: One can use $\frac{d^3\boldsymbol{P}_a}{2E_a} = d^4P_a\,\delta\big((P_a)^2 + m_\phi^2\big)\,\theta\big(P_a^0\big)$ and integrate over d^4P_2 to get

$$\frac{P}{T_{\text{out}} - T_{\text{in}}} = \frac{\kappa^2}{4E_0}\int\frac{d^4P_1}{(2\pi)^3}\delta\big((P_1)^2 + m_\phi^2\big)\,\theta(E_1)\,\frac{1}{(2\pi)^3}\delta\big((P_0 - P_1)^2 + m_\phi^2\big)\,\theta(E_0 - E_1)\,(2\pi)^4$$
$$= \frac{\kappa^2}{4E_0}2\pi\int_0^\infty\frac{p_1^2dp_1}{(2\pi)^6\,2E_1}\int_{-1}^1 d\cos\theta\,\delta\big(2E_0E_1 - 2p_0p_1\cos\theta - m_\Phi^2\big)\,\theta(E_0 - E_1)\,(2\pi)^4$$
$$= \frac{\kappa^2}{4E_0}2\pi\int_{-1\le\frac{2E_0E_1 - m_\Phi^2}{2p_0p_1}\le 1}\frac{p_1^2dp_1}{(2\pi)^6\,2E_1}\frac{1}{2p_0p_1}\theta(E_0 - E_1)\,(2\pi)^4\,,$$

where $p_1 = |\boldsymbol{P}_1|$, $E_1 = \sqrt{p_1^2 + m_\phi^2}$, and $p_0 = |\boldsymbol{P}_0| = \sqrt{E_0^2 - m_\Phi^2}$. One may perform the integral in the last line by $p_1dp_1 = E_1dE_1$ to obtain Eq. (105).

[23] It should be understood that the limit $\sigma_t \to 0$ is taken with fixed $\sqrt{\sigma_t}\delta\omega$.

We may further take the plane-wave limit $\sigma_s \to \infty$, which renders the factor in the square brackets into the delta function $\delta^3(\delta \boldsymbol{P})$:

$$dP = \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\,2E_1}\frac{1}{(2\pi)^3\,2E_2}(2\pi)^4\,\frac{2}{\pi}\frac{1}{(\delta E)^2}, \tag{109}$$

where we have also replaced $\delta\omega$ by δE; see Eq. (37). We see that the ultraviolet behavior of the momentum integral is

$$dP \propto \int \frac{d\,|\boldsymbol{P}_1|}{|\boldsymbol{P}_1|^2}, \tag{110}$$

which is convergent. This convergence itself is independent of the limits that we have taken.

There is no ultraviolet divergence from the boundary regions if the decay is due to the superrenormalizable interaction of Eq. (1). In contrast, if the decay of scalar were due to a marginal operator of dimension four, we would have got a linearly divergent integral instead of Eq. (110).[24]

We comment on the possible ultraviolet divergence at the boundary. First, one might want to take into account the "uncertainty" of $T_{\text{in/out}}$ that is defined in our treatment to be the time (at which the interacting state can well be identified with the free state), by "diffusing the boundary" à la Stueckelberg [12]. This would provide an additional UV suppression factor on the momentum integral, but the necessary unitarity violation requires the change of the very definition of the S-matrix. Second, as stated in footnote 17, the identification of the interacting state with the free state at $T_{\text{in/out}}$ cannot be justified for the boundary contribution. Third, in realistic (particle physics) situations, there is no ideally sharp time boundary but some production and detection mechanisms that are extended in spacetime. The phenomenology on the boundary region could strongly depend on the microscopic physics of the boundary. Thus, the boundary contribution depends on the situation or might not be valid when it is ultraviolet divergent. Further discussion and the implications will be presented elsewhere.

5. Diphoton decay

In order to exhibit how to generalize the simplest scalar decay by the interaction in Eq. (1) to more realistic cases, we consider the decay of a pseudoscalar into a diphoton pair:

$$\mathcal{L}_{\text{int}} = -\frac{g_\Phi}{4}\Phi\varepsilon_{\lambda\mu\nu\rho}F^{\lambda\mu}F^{\nu\rho} = -\mathcal{H}_{\text{int}}, \tag{111}$$

where $\varepsilon^{\lambda\mu\nu\rho}$ is the totally antisymmetric tensor and g_Φ is a coupling constant of mass dimension -1. For the pion decay, we set $g_\Phi = \frac{\sqrt{2}\alpha}{\pi f_\pi}$, where $\alpha \simeq 1/137$ and $f_\pi \simeq 130\,\text{MeV}$ are the fine structure and pion decay constants, respectively.

It is actually straightforward to generalize the previous analysis to the diphoton decay. The photon field operator can be expanded in terms of the creation/annihilation operators of the plane and Gaussian waves as

$$\hat{A}_\mu(x) = \sum_s \int \frac{d^3\boldsymbol{p}}{\sqrt{2p^0}\,(2\pi)^{3/2}}\left[\hat{a}(s,\boldsymbol{p})\,\epsilon_\mu(s,\boldsymbol{p})\,e^{ip\cdot x} + \hat{a}^\dagger(s,\boldsymbol{p})\,\epsilon^*_\mu(s,\boldsymbol{p})\,e^{-ip\cdot x}\right]\Bigg|_{p^0=|\boldsymbol{p}|} \tag{112}$$

[24] Naively, dimensional analysis tells that the tree-level two-body decay of a scalar due to a dimension-d operator would result in ultraviolet divergence of the order of $2d-7$. This is the case for the non-renormalizable interaction in Eq. (111) too.

$$= \sum_s \int \frac{d^3\boldsymbol{X} d^3\boldsymbol{P}}{(2\pi)^3} \left[E_\mu(s,\sigma;X,\boldsymbol{P})\,\hat{A}(s,\sigma;X,\boldsymbol{P}) + E_\mu^*(s,\sigma;X,\boldsymbol{P})\,\hat{A}^\dagger(s,\sigma;X,\boldsymbol{P}) \right], \quad (113)$$

respectively, where

$$E_\mu(s,\sigma;X,\boldsymbol{P}) = \int \frac{d^3\boldsymbol{p}}{\sqrt{2p^0}} \epsilon_\mu(s,\boldsymbol{p})\, e^{ip\cdot(x-X)-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\bigg|_{p^0=|\boldsymbol{p}|}; \quad (114)$$

see Appendix A.3. The saddle-point approximation in the large-width expansion gives[25]

$$E_\mu(s,\sigma;X,\boldsymbol{P}) \simeq \left(\frac{\sigma}{\pi}\right)^{4/3} \left(\frac{2\pi}{\sigma}\right)^{3/2} \left(\frac{1}{(2\pi)^3\, 2\,|\boldsymbol{P}|}\right)^{1/2} \epsilon_\mu(s,\boldsymbol{P})\, e^{-i|\boldsymbol{P}|(t-T)+i\boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{X})-\frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t))^2}{2\sigma}}; \quad (115)$$

see Appendix B.

In obtaining the S-matrix, all we have to do is to replace κ by

$$\kappa \mapsto g_\Phi\, \varepsilon_{\lambda\mu\nu\rho} P_1^\lambda \epsilon^{\mu*}(s_1,\boldsymbol{P}_1)\, P_2^\nu \epsilon^{\rho*}(s_2,\boldsymbol{P}_2) \quad (116)$$

in Eq. (58). The spin-summed decay probability is then, from Eq. (85),

$$dP = \frac{2g_\Phi^2\,(P_1\cdot P_2)^2}{2} \frac{1}{2E_0} \frac{d^3\boldsymbol{P}_1}{(2\pi)^3\, 2E_1} \frac{d^3\boldsymbol{P}_2}{(2\pi)^3\, 2E_2} (2\pi)^4 \left(\sqrt{\frac{\sigma_t}{\pi}} e^{-\sigma_t(\delta\omega)^2}\right) \left(\left(\frac{\sigma_s}{\pi}\right)^{3/2} e^{-\sigma_s(\delta\boldsymbol{P})^2}\right)$$
$$\times \sqrt{\frac{\sigma_t}{\pi^5}\left(\frac{\sigma_s}{\sigma_0\sigma_1\sigma_2}\right)^3}\, d^3\boldsymbol{X}_1\, d^3\boldsymbol{X}_2\, e^{-\mathcal{R}}\, |G(\mathfrak{T})|^2, \quad (117)$$

where we have used

$$\sum_{s_1,s_2} \left|\varepsilon_{\lambda\mu\nu\rho} P_1^\lambda \epsilon^\mu(s_1,\boldsymbol{P}_1)\, P_2^\nu \epsilon^\rho(s_2,\boldsymbol{P}_2)\right|^2 = 2\,(P_1\cdot P_2)^2. \quad (118)$$

After taking the plane-wave limit, the final expression for Fermi's golden rule, Eq. (104), becomes

$$\frac{dP}{T_{\text{out}}-T_{\text{in}}} = \frac{g_\Phi^2 m_\Phi^4}{8E_0} \left(\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\, 2E_1}\right) \left(\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\, 2E_2}\right) (2\pi)^4\, \delta^4(P_1+P_2-P_0), \quad (119)$$

where we used, under the momentum delta function and the on-shell condition,

$$P_1\cdot P_2 = \frac{(P_1+P_2)^2}{2} = \frac{P_0^2}{2} = -\frac{m_\Phi^2}{2}. \quad (120)$$

The total decay rate is

$$\frac{P}{T_{\text{out}}-T_{\text{in}}} = \frac{g_\Phi^2 m_\Phi^4}{64\pi E_0}. \quad (121)$$

That is, the replacement in the final expression reads $\kappa^2 \mapsto g_\Phi^2 m_\Phi^4/2$ (and of course $m_\phi \mapsto 0$).

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[25] One can explicitly check that the next-to-leading-order terms in the expansion in Eq. (B.19) cancel out in the final expression of the probability dP. For example, the saddle-point momentum remains massless at the next-to-leading order: $\left(\boldsymbol{P} \pm i\frac{\boldsymbol{x}-\boldsymbol{\Xi}(t)}{\sigma}\right)^2 = \boldsymbol{P}^2 + \mathcal{O}\left(\frac{1}{\sigma^2}\right)$.

6. Summary

We have reformulated the Gaussian S-matrix within a finite time interval in the Gaussian wave-packet formalism. The normalizable Gaussian basis allows the computation of the decay probability without the momentum-space $\delta^4(0)$ singularity that necessarily appears in the one involving the plane-wave basis. We have performed the exact four-dimensional integration over the interaction point x for the decay probability. The unitarity is manifestly maintained throughout the whole computation.

We have proposed a separation of the obtained result into the bulk and boundary parts. This separation corresponds to whether the interaction point is near the time boundary or not and hence is rather intuitive and easy to envisage. Fermi's golden rule is derived from the bulk contribution. As a byproduct, we have also shown that the ultraviolet divergence in the boundary contribution is absent for the decay of a scalar into a pair of light scalars by the superrenormalizable interaction, though its physical significance is yet to be confirmed. We have generalized our results to the case of diphoton decay and to more general initial and final state particles.

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Appendix A. Gaussian wave packet formalism

We review and spell out our notation for the Gaussian wave-packet basis [3,8,11].

A.1. Heisenberg, Schrödinger, and interaction pictures

We may always separate the total Lagrangian density $\mathcal{L}$ into the free part $\mathcal{L}_{\text{free}}$ that contains quadratic terms in fields and the interaction one $\mathcal{L}_{\text{int}}$ that is the rest:

$$\mathcal{L} = \mathcal{L}_{\text{free}} + \mathcal{L}_{\text{int}}. \tag{A.1}$$

Correspondingly, we may separate the Hamiltonian (density) H ($\mathcal{H}$) into the free and interaction parts H_{free} ($\mathcal{H}_{\text{free}}$) and H_{int} ($\mathcal{H}_{\text{int}}$), respectively:

$$H = H_{\text{free}} + H_{\text{int}}, \qquad \mathcal{H} = \mathcal{H}_{\text{free}} + \mathcal{H}_{\text{int}}. \tag{A.2}$$

We list the time dependence of the physical state, operator, and eigenbasis in the Heisenberg, Schrödinger, and interaction pictures in the Table A1.[26]

Throughout this paper, $\hat{H}$ ($\hat{H}_{\text{free}}$) denotes the time-independent total (free) Hamiltonian in the Schrödinger or Heisenberg (interaction) picture. Any Schrödinger eigenbasis $|\Phi\rangle^{(\text{SB})}$ can be regarded as a Heisenberg state:

$$|\Phi\rangle^{(\text{SB})} = |\Phi\rangle^{(\text{H})}. \tag{A.3}$$

[26] We choose our reference time to identify these three pictures to be $t = 0$ throughout this paper.

Table A1. Time dependences in the different pictures.

Picture	State	Operator	Basis
Heisenberg	$\lvert\Phi\rangle^{(\mathrm{H})}$	$\hat{O}^{(\mathrm{H})}(t)=e^{i\hat{H}t}\hat{O}^{(\mathrm{S})}e^{-i\hat{H}t}$	$\lvert\Phi,t\rangle^{(\mathrm{HB})}=e^{i\hat{H}t}\lvert\Phi\rangle^{(\mathrm{SB})}$
Schrödinger	$\lvert\Phi,t\rangle^{(\mathrm{S})}=e^{-i\hat{H}t}\lvert\Phi\rangle^{(\mathrm{H})}$	$\hat{O}^{(\mathrm{S})}$	$\lvert\Phi\rangle^{(\mathrm{SB})}$
Interaction	$\lvert\Phi,t\rangle^{(\mathrm{I})}=e^{i\hat{H}_{\mathrm{free}}t}e^{-i\hat{H}t}\lvert\Phi\rangle^{(\mathrm{H})}$	$\hat{O}^{(\mathrm{I})}(t)=e^{i\hat{H}_{\mathrm{free}}t}\hat{O}^{(\mathrm{S})}e^{-i\hat{H}_{\mathrm{free}}t}$	$\lvert\Phi,t\rangle^{(\mathrm{IB})}=e^{i\hat{H}_{\mathrm{free}}t}\lvert\Phi\rangle^{(\mathrm{SB})}$

A.2. Plane-wave expansion

Let us spell out the ordinary plane-wave basis as a preparation for the Gaussian basis.

A free field operator $\hat{\Psi}^{(\mathrm{I})}(x)$ at $x=\left(x^0,\boldsymbol{x}\right)=(t,\boldsymbol{x})$ in the interaction picture can be expanded in terms of the plane waves $e^{\pm ip\cdot x}$:

$$\hat{\Psi}^{(\mathrm{I})}(x)=\sum_s\int\frac{d^3\boldsymbol{p}}{\sqrt{2p^0}\,(2\pi)^{3/2}}\left[\hat{a}_\Psi(s,\boldsymbol{p})\,U(s,\boldsymbol{p})\,e^{ip\cdot x}+\hat{a}^{c\dagger}_\Psi(s,\boldsymbol{p})\,V(s,\boldsymbol{p})\,e^{-ip\cdot x}\right]\Bigg|_{p^0=E_\Psi(\boldsymbol{p})}, \tag{A.4}$$

where $E_\Psi(\boldsymbol{p})$ is given in Eq. (3); s is the helicity or the spin (of the little group); and the coefficient functions U and V are given, e.g., for a scalar ($s=0$), a Dirac spinor ($s=\pm1/2$), and a massless vector ($s=\pm1$) as[27]

$$U(s,\boldsymbol{p})=\begin{cases}1,\\ u(s,\boldsymbol{p}),\\ \epsilon_\mu(s,\boldsymbol{p}),\end{cases}\qquad V(s,\boldsymbol{p})=\begin{cases}1,\\ v(s,\boldsymbol{p}),\\ \epsilon^*_\mu(s,\boldsymbol{p}),\end{cases}\qquad\text{for}\qquad \hat{\Psi}^{(\mathrm{I})}(x)=\begin{cases}\hat{\varphi}(x) & \text{(scalar)},\\ \hat{\psi}(x) & \text{(spinor)},\\ \hat{A}_\mu(x) & \text{(vector)}.\end{cases} \tag{A.5}$$

Here and hereafter, the annihilation operators $\hat{a}$ and $\hat{a}^c$ are always given in the Schrödinger picture (i.e. independent of time) as usual. The creation and annihilation operators obey

$$\begin{aligned}\left[\hat{a}_\Psi(s,\boldsymbol{p}),\hat{a}^\dagger_{\Psi'}(s',\boldsymbol{p}')\right]_\pm&=\delta_{\Psi\Psi'}\delta_{ss'}\delta^3\left(\boldsymbol{p}-\boldsymbol{p}'\right),\\ \left[\hat{a}^c_\Psi(s,\boldsymbol{p}),\hat{a}^{c\dagger}_{\Psi'}(s',\boldsymbol{p}')\right]_\pm&=\delta_{\Psi\Psi'}\delta_{ss'}\delta^3\left(\boldsymbol{p}-\boldsymbol{p}'\right),\\ \text{others}&=0,\end{aligned} \tag{A.6}$$

where the plus and minus signs correspond to the anticommutator and commutator when both Ψ and Ψ' are fermions ($s=\pm1/2$) and otherwise, respectively. A real (Majorana) field corresponds to $\hat{a}^c(s,\boldsymbol{p})=\hat{a}(s,\boldsymbol{p})$.

A free massless (massive) one-particle state with a definite helicity (spin) s and momentum $\boldsymbol{p}$ is given by

$$\lvert s,\boldsymbol{p}\rangle^{(\mathrm{SB})}_\Psi=\hat{a}^\dagger_\Psi(s,\boldsymbol{p})\,\lvert0\rangle, \tag{A.7}$$

where we have normalized such that

$${}^{(\mathrm{SB})}_{\quad\Psi}\langle s,\boldsymbol{p}\,|\,s',\boldsymbol{p}'\rangle^{(\mathrm{SB})}_{\Psi'}=\delta^3\left(\boldsymbol{p}-\boldsymbol{p}'\right)\delta_{ss'}\delta_{\Psi\Psi'},\qquad\int d^3\boldsymbol{p}\,\lvert s,\boldsymbol{p}\rangle^{(\mathrm{SB})}_\Psi\,{}^{(\mathrm{SB})}_{\quad\Psi}\langle s,\boldsymbol{p}\rvert=\hat{1}, \tag{A.8}$$

[27] The dependence of u and v on the mass m_Ψ is made implicit.

where $\hat{1}$ is the identity operator in the one-particle subspace with a definite s. One obtains the free Hamiltonian

$$\hat{H}_{\text{free}} = \sum_{\Psi}\sum_{s}\int d^3\boldsymbol{p}\, E_\Psi(\boldsymbol{p})\, \hat{a}^\dagger_\Psi(s,\boldsymbol{p})\, \hat{a}_\Psi(s,\boldsymbol{p}) \tag{A.9}$$

up to a constant term, and the state in Eq. (A.7) becomes the eigenbasis for it:

$$\hat{H}_{\text{free}}\, |s,\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi} = E_\Psi(\boldsymbol{p})\, |s,\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi}. \tag{A.10}$$

As in the ordinary quantum mechanics, the one-particle position eigenbasis ${}^{(\text{SB})}_{\Psi}\langle s,\boldsymbol{x}|$ is defined to yield the plane-wave function when multiplied on $|s,\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi}$:

$${}^{(\text{SB})}_{\Psi}\langle s,\boldsymbol{x}\,|\,s',\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi'} = \frac{e^{i\boldsymbol{p}\cdot\boldsymbol{x}}}{(2\pi)^{3/2}}\delta_{ss'}\delta_{\Psi\Psi'}, \tag{A.11}$$

where its normalization is chosen such that

$${}^{(\text{SB})}_{\Psi}\langle s,\boldsymbol{x}\,|\,s',\boldsymbol{x}'\rangle^{(\text{SB})}_{\Psi'} = \delta^3\left(\boldsymbol{x}-\boldsymbol{x}'\right)\delta_{ss'}\delta_{\Psi\Psi'}, \qquad \int d^3\boldsymbol{x}\ |s,\boldsymbol{x}\rangle^{(\text{SB})}_{\Psi}\ {}^{(\text{SB})}_{\Psi}\langle s,\boldsymbol{x}| = \hat{1}. \tag{A.12}$$

We may call the position eigenbasis in the interaction picture at time t "the time-translated position eigenbasis at $x = \left(x^0,\boldsymbol{x}\right) = (t,\boldsymbol{x})$":

$${}^{(\text{IB})}_{\Psi}\langle s,x| := {}^{(\text{SB})}_{\Psi}\langle s,\boldsymbol{x}|\, e^{-i\hat{H}_{\text{free}}t}. \tag{A.13}$$

Concretely, we get

$${}^{(\text{IB})}_{\Psi}\langle s,x\,|\,s',\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi} = \left.\frac{e^{ip\cdot x}}{(2\pi)^{3/2}}\right|_{p^0=E_\Psi(\boldsymbol{p})}\delta_{ss'}. \tag{A.14}$$

The completeness still holds,

$$\int d^3\boldsymbol{x}\, |s,x\rangle^{(\text{IB})}_{\Psi}\ {}^{(\text{IB})}_{\Psi}\langle s,x| = \hat{1}, \tag{A.15}$$

whereas the orthogonality holds only at the equal time:

$$\left.{}^{(\text{IB})}_{\Psi}\langle s,x\,|\,s',x'\rangle^{(\text{IB})}_{\Psi'}\right|_{t=t'} = \delta^3\left(\boldsymbol{x}-\boldsymbol{x}'\right)\delta_{ss'}\delta_{\Psi\Psi'}. \tag{A.16}$$

Now we may rewrite:

$$\hat{\Psi}^{(\text{I})}(x) = \sum_s\int\frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}} \times\left[\hat{a}(s,\boldsymbol{p})\,U(s,\boldsymbol{p})\left({}^{(\text{IB})}_{\Psi}\langle s,x\,|\,s,\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi}\right) + \hat{a}^{c\dagger}(s,\boldsymbol{p})\,V(s,\boldsymbol{p})\left({}^{(\text{IB})}_{\Psi}\langle s,x\,|\,s,\boldsymbol{p}\rangle^{(\text{SB})}_{\Psi}\right)^*\right]. \tag{A.17}$$

A.3. Gaussian wave packets

We define a free Gaussian wave-packet state $|s,\sigma;\boldsymbol{X},\boldsymbol{P}\rangle^{(\text{SB})}_{\Psi}$ that is localized at $\boldsymbol{X}$ with width $\sqrt{\sigma}$ and central momentum $\boldsymbol{P}$ by the standard Gaussian wave function of $\boldsymbol{x}$:

$${}^{(\text{SB})}_{\Psi}\langle s,\boldsymbol{x}\,|\,s',\sigma;\boldsymbol{X},\boldsymbol{P}\rangle^{(\text{SB})}_{\Psi} = \frac{1}{(\pi\sigma)^{3/4}}e^{i\boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{X})}e^{-\frac{1}{2\sigma}(\boldsymbol{x}-\boldsymbol{X})^2}\delta_{ss'}, \tag{A.18}$$

where we have normalized such that

$$\int d^3\boldsymbol{x} \left| {}^{(\mathrm{SB})}_{\ \ \Psi}\langle s, \boldsymbol{x} \,|\, s, \sigma; \boldsymbol{X}, \boldsymbol{P}\rangle^{(\mathrm{SB})}_{\Psi} \right|^2 = 1. \tag{A.19}$$

Analogously to the plane-wave basis in Eq. (A.13), we may define the Gaussian basis that is centered at $X = \left(X^0, \boldsymbol{X}\right) = (T, \boldsymbol{X})$ by

$${}^{(\mathrm{IB})}_{\ \ \Psi}\langle s, \sigma; X, \boldsymbol{P}| := {}^{(\mathrm{SB})}_{\ \ \Psi}\langle s, \sigma; \boldsymbol{X}, \boldsymbol{P}|\, e^{-i\hat{H}_{\mathrm{free}}T}. \tag{A.20}$$

Concretely, we obtain

$${}^{(\mathrm{IB})}_{\ \ \Psi}\langle s, \sigma; X, \boldsymbol{P} \,|\, s, \boldsymbol{p}\rangle^{(\mathrm{SB})} = \left(\frac{\sigma}{\pi}\right)^{3/4} e^{ip\cdot X} e^{-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\Big|_{p^0=E_\Psi(\boldsymbol{p})}, \tag{A.21}$$

where we have used Eqs. (A.14) and (A.18).[28] Note that the completeness relation now becomes[29]

$$\int \frac{d^3\boldsymbol{X}\, d^3\boldsymbol{P}}{(2\pi)^3}\, |s, \sigma; X, \boldsymbol{P}\rangle^{(\mathrm{IB})}_{\Psi}\ {}^{(\mathrm{IB})}_{\ \ \Psi}\langle s, \sigma; X, \boldsymbol{P}| = \hat{1} \tag{A.22}$$

and that the Gaussian basis states are not orthogonal to each other even if $T = T'$:

$$\begin{aligned} &{}^{(\mathrm{IB})}_{\ \ \Psi}\!\left\langle s, \sigma; X, \boldsymbol{P} \,\middle|\, s', \sigma'; X', \boldsymbol{P}'\right\rangle^{(\mathrm{IB})}_{\Psi'} \Big|_{T=T'} \\ &= \left(\frac{\sigma_{\mathrm{I}}}{\sigma_{\mathrm{A}}}\right)^{3/4} e^{-\frac{1}{4\sigma_{\mathrm{A}}}(\boldsymbol{X}-\boldsymbol{X}')^2} e^{-\frac{\sigma_{\mathrm{I}}}{4}(\boldsymbol{P}-\boldsymbol{P}')^2} e^{\frac{i}{2\sigma_{\mathrm{I}}}(\sigma\boldsymbol{P}+\sigma'\boldsymbol{P}')\cdot(\boldsymbol{X}-\boldsymbol{X}')}\, \delta_{ss'}\delta_{\Psi\Psi'}, \end{aligned} \tag{A.23}$$

where $\sigma_{\mathrm{A}} := \frac{\sigma+\sigma'}{2}$ and $\sigma_{\mathrm{I}} := \left(\frac{\sigma^{-1}+\sigma'^{-1}}{2}\right)^{-1} = \frac{2\sigma\sigma'}{\sigma+\sigma'}$ are the average and the inverse of inverse average, respectively. Namely, the Gaussian basis is overcomplete.

Now we define the creation operator of the free wave packet $\hat{A}^\dagger_\Psi(s, \sigma; X, \boldsymbol{P})$ by[30]

$$\hat{A}^\dagger_\Psi(s, \sigma; X, \boldsymbol{P})\,|0\rangle = |s, \sigma; X, \boldsymbol{P}\rangle^{(\mathrm{IB})}_{\Psi}, \tag{A.24}$$

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[28] Though not quite useful, we may also write down the time-shifted Gaussian wave function in an integral form:

$${}^{(\mathrm{IB})}_{\ \ \Psi}\langle s, x \,|\, s, \sigma; X, \boldsymbol{P}\rangle^{(\mathrm{IB})}_{\Psi} = \left(\frac{\sigma}{\pi}\right)^{3/4} \int \frac{d^3\boldsymbol{p}}{(2\pi)^{3/2}}\, e^{ip\cdot(x-X)-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\Big|_{p^0=E_\Psi(\boldsymbol{p})}.$$

[29] One can explicitly show that

$$\langle \boldsymbol{p}| \left(\int \frac{d^3\boldsymbol{X}\, d^3\boldsymbol{P}}{(2\pi)^3}\, |\sigma; X, \boldsymbol{P}\rangle\, \langle \sigma; X, \boldsymbol{P}|\right) \left|\boldsymbol{p}'\right\rangle = \delta^3\!\left(\boldsymbol{p} - \boldsymbol{p}'\right),$$

where we have tentatively omitted Ψ, s, etc.

[30] We note that, in the Gaussian formulation, the postulation (c) in Ref. [15] does not hold, nor its conclusion of no-go, because the Gaussian basis states are not orthogonal to each other even when their locations $\boldsymbol{X}$ and $\boldsymbol{X}'$ are different, as can be seen in Eq. (A.23). We thank Akio Hosoya and Izumi Ojima for pointing out this issue.

which leads to[31]

$$\hat{A}_\Psi(s,\sigma;X,\boldsymbol{P}) = \int d^3\boldsymbol{p}\left({}^{\text{(IB)}}_{\ \ \Psi}\langle s,\sigma;X,\boldsymbol{P}\,|\,s;\boldsymbol{p}\rangle^{\text{(SB)}}_{\Psi}\right)\hat{a}_\Psi(s,\boldsymbol{p}), \tag{A.25}$$

$$\hat{a}_\Psi(s,\boldsymbol{p}) = \int\frac{d^3\boldsymbol{X}d^3\boldsymbol{P}}{(2\pi)^3}\left({}^{\text{(SB)}}_{\ \ \Psi}\langle s,\boldsymbol{p}\,|\,s,\sigma;X,\boldsymbol{P}\rangle^{\text{(IB)}}_{\Psi}\right)\hat{A}_\Psi(s,\sigma;X,\boldsymbol{P}). \tag{A.26}$$

Note that

$$\left[\hat{A}_\Psi(s,\sigma;X,\boldsymbol{P}),\hat{A}^\dagger_{\Psi'}\left(s',\sigma';X',\boldsymbol{P}'\right)\right]_\pm = {}^{\text{(IB)}}_{\ \ \Psi}\langle s',\sigma;X,\boldsymbol{P}\,|\,s,\sigma';X',\boldsymbol{P}'\rangle^{\text{(IB)}}_{\Psi'},$$

$$\text{others} = 0. \tag{A.27}$$

To obtain the explicit form of the expansion in terms of the Gaussian basis, one may put Eq. (A.26) into Eq. (A.17):

$$\hat{\Psi}^{(\text{I})}(x) = \sum_s\int\frac{d^3\boldsymbol{X}d^3\boldsymbol{P}}{(2\pi)^3}\left[\mathcal{U}_{s,\sigma;X,\boldsymbol{P}}(x)\,\hat{A}_\Psi(s,\sigma;X,\boldsymbol{P}) + \mathcal{V}_{s,\sigma;X,\boldsymbol{P}}(x)\,\hat{A}^{c\dagger}_\Psi(s,\sigma;X,\boldsymbol{P})\right], \tag{A.28}$$

where

$$\mathcal{U}_{s,\sigma;X,\boldsymbol{P}}(x) := \int\frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}}\left({}^{\text{(IB)}}_{\ \ \Psi}\langle s,x\,|\,s,\boldsymbol{p}\rangle^{\text{(SB)}}_{\Psi}\right)U(s,\boldsymbol{p})\left({}^{\text{(SB)}}_{\ \ \Psi}\langle s,\boldsymbol{p}\,|\,s,\sigma;X,\boldsymbol{P}\rangle^{\text{(IB)}}_{\Psi}\right), \tag{A.29}$$

$$\mathcal{V}_{s,\sigma;X,\boldsymbol{P}}(x) := \int\frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}}\left({}^{\text{(IB)}}_{\ \ \Psi}\langle s,\sigma;X,\boldsymbol{P}\,|\,s,\boldsymbol{p}\rangle^{\text{(SB)}}_{\Psi}\right)V(s,\boldsymbol{p})\left({}^{\text{(SB)}}_{\ \ \Psi}\langle s,\boldsymbol{p}\,|\,s,x\rangle^{\text{(IB)}}_{\Psi}\right). \tag{A.30}$$

Using Eqs. (A.14) and (A.21), one may write down the integral form more explicitly:

$$\mathcal{U}_{s,\sigma;X,\boldsymbol{P}}(x) = \left(\frac{\sigma}{\pi}\right)^{3/4}\int\frac{d^3\boldsymbol{p}}{\sqrt{2p^0}\,(2\pi)^{3/2}}U(s,\boldsymbol{p})\,e^{ip\cdot(x-X)-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\bigg|_{p^0=E_\Psi(\boldsymbol{p})}, \tag{A.31}$$

$$\mathcal{V}_{s,\sigma;X,\boldsymbol{P}}(x) = \left(\frac{\sigma}{\pi}\right)^{3/4}\int\frac{d^3\boldsymbol{p}}{\sqrt{2p^0}\,(2\pi)^{3/2}}V(s,\boldsymbol{p})\,e^{-ip\cdot(x-X)-\frac{\sigma}{2}(\boldsymbol{p}-\boldsymbol{P})^2}\bigg|_{p^0=E_\Psi(\boldsymbol{p})}. \tag{A.32}$$

Note that T $(=X^0)$ and σ can be chosen arbitrarily for the expansion in Eq. (A.28). The coefficient functions $\mathcal{U}$ and $\mathcal{V}$ are nothing but the external line factor in the computation of S-matrix:

$$\begin{aligned}\langle 0|\,\hat{\Psi}^{(\text{I})}(x)\,|s,\sigma;X,\boldsymbol{P}\rangle^{\text{(IB)}}_{\Psi} &= \sum_s\int d^6\boldsymbol{\Pi}'\,\mathcal{U}_{s;\Pi'}(x)\;\langle 0|\,\hat{A}_\Psi\left(s;\Pi'\right)\hat{A}^\dagger_\Psi(s;\Pi)\,|0\rangle\\ &= \sum_s\int d^6\boldsymbol{\Pi}'\left(\int\frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}}\,\langle x\,|\,\boldsymbol{p}\rangle\,U(\boldsymbol{p})\left\langle\boldsymbol{p}\,|\,\Pi'\right\rangle\right)\left\langle\Pi'\,|\,\Pi\right\rangle\end{aligned}$$

[31] When we expand $\hat{A}$ by $\hat{a}$ as $\hat{A}(\sigma;X,\boldsymbol{P}) = \int d^3\boldsymbol{p}'\,f_{\boldsymbol{p}'}(\sigma;X,\boldsymbol{P})\;\hat{a}(\boldsymbol{p}')$ (we have omitted Ψ, s, etc.), we get

$$\langle 0|\,\hat{A}(\sigma;X,\boldsymbol{P})\,|\boldsymbol{p}\rangle = \langle 0|\int d^3\boldsymbol{p}'\,f_{\boldsymbol{p}'}(\sigma;X,\boldsymbol{P})\;\hat{a}\left(\boldsymbol{p}'\right)|\boldsymbol{p}\rangle = f_{\boldsymbol{p}}(\sigma;X,\boldsymbol{P}),$$

which is equated to Eq. (A.21) to yield Eq. (A.25).

$$= \sum_s \int \frac{d^3\boldsymbol{p}}{\sqrt{2E_\Psi(\boldsymbol{p})}} \langle x \,|\, \boldsymbol{p} \rangle \, U(\boldsymbol{p}) \, \langle \boldsymbol{p} \,|\, \Pi \rangle$$

$$= \mathcal{U}_{s,\sigma;X,\boldsymbol{P}}(x)\,, \tag{A.33}$$

and so on, where we have omitted Ψ, σ, and s in the intermediate steps and have used the abbreviation in Eq. (15).

Appendix B. Saddle-point approximation

Let us obtain the approximate formulae for the functions in Eqs. (A.31) and (A.32) using the saddle-point method for the large-width expansion. When evaluating the momentum integration, we encounter the exponent of the form[32]

$$F_\pm(\boldsymbol{p}) := \mp iE(\boldsymbol{p})\,(t-T) \pm i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{X}) - \frac{\sigma}{2}\,(\boldsymbol{p}-\boldsymbol{P})^2\,, \tag{B.1}$$

where $E(\boldsymbol{p}) := \sqrt{\boldsymbol{p}^2+m^2}$. First,

$$\frac{\partial F_\pm(\boldsymbol{p})}{\partial p_i} = \mp i v_i(\boldsymbol{p})\,(t-T) \pm i\,(x-X)_i - \sigma\,(p-P)_i\,, \tag{B.2}$$

$$\frac{\partial^2 F_\pm(\boldsymbol{p})}{\partial p_i \partial p_j} = \mp i \frac{t-T}{E(\boldsymbol{p})}\left[\delta_{ij} - v_i(\boldsymbol{p})\,v_j(\boldsymbol{p})\right] - \sigma\delta_{ij}, \tag{B.3}$$

where

$$\boldsymbol{v}(\boldsymbol{p}) := \frac{\boldsymbol{p}}{E(\boldsymbol{p})} \tag{B.4}$$

and we have used

$$\frac{\partial E(\boldsymbol{p})}{\partial p_j} = v_j(\boldsymbol{p})\,, \qquad \frac{\partial v_i(\boldsymbol{p})}{\partial p_j} = \frac{\delta_{ij} - v_i(\boldsymbol{p})\,v_j(\boldsymbol{p})}{E(\boldsymbol{p})}. \tag{B.5}$$

Let $\boldsymbol{P}_s$ be the solution to the saddle-point condition:

$$\frac{\partial F_\pm(\boldsymbol{P}_s)}{\partial p_i} = 0, \tag{B.6}$$

where for arbitrary $\boldsymbol{P}$ and function $f(\boldsymbol{p})$, we write

$$\frac{\partial f(\boldsymbol{P})}{\partial p_i} := \left.\frac{\partial f(\boldsymbol{p})}{\partial p_i}\right|_{\boldsymbol{p}=\boldsymbol{P}}. \tag{B.7}$$

The zeroth and second derivatives read

$$F_\pm(\boldsymbol{P}_s) = \mp iE(\boldsymbol{P}_s)\,(t-T) \pm i\boldsymbol{P}_s\cdot(\boldsymbol{x}-\boldsymbol{X}) - \frac{\sigma}{2}\,(\boldsymbol{P}_s-\boldsymbol{P})^2\,, \tag{B.8}$$

$$\frac{\partial^2 F_\pm(\boldsymbol{P}_s)}{\partial p_i \partial p_j} = -\left(\sigma \pm i\frac{t-T}{E(\boldsymbol{P}_s)}\right)\delta_{ij} \pm i\frac{t-T}{E(\boldsymbol{P}_s)} v_i(\boldsymbol{P}_s)\,v_j(\boldsymbol{P}_s) =: M_{ij}. \tag{B.9}$$

[32] In taking the large-σ expansion, we have to be careful about the region of large $|\boldsymbol{x}-\boldsymbol{X}|$ and/or large $|t-T|$. Here we assume that we are in a generic non-singular point in the parameter space in which the contribution from such an interaction point x is suppressed and that the large-σ expansion works.

The complex symmetric matrix $M_{ij} = a\delta_{ij} + b v_j v_j$ can be diagonalized by a complex special orthogonal matrix U that obeys $U^{\rm t} U = 1$ and $\det U = 1$:[33]

$$U^{\rm t} M U = \begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a + b\boldsymbol{v}^2 \end{bmatrix}. \tag{B.10}$$

The complex Gaussian integral reads

$$\int d^3 p\, e^{F_\pm(\boldsymbol{p})} Q(\boldsymbol{p}) \simeq e^{F(\boldsymbol{P}_s)} Q(\boldsymbol{P}_s) \int d^3 p\, e^{\frac{1}{2}(p-P_s)_i \frac{\partial^2 F(\boldsymbol{P}_s)}{\partial p_i \partial p_j}(p-P_s)_j}$$
$$= \left(\frac{2\pi}{\sigma}\right)^{3/2} \frac{e^{F(\boldsymbol{P}_s)} Q(\boldsymbol{P}_s)}{\left(1 \pm i\frac{t-T}{\sigma E(\boldsymbol{P}_s)}\right)\sqrt{1 \pm i\frac{t-T}{\sigma E(\boldsymbol{P}_s)}\left(1 - \boldsymbol{v}^2(\boldsymbol{P}_s)\right)}}, \tag{B.11}$$

for any polynomial $Q(\boldsymbol{p})$. Note that the Gaussian integral can be performed when

$$1 > \mp \Im \frac{t-T}{\sigma E(\boldsymbol{P}_s)} = \pm \frac{t-T}{\sigma\, |E(\boldsymbol{P}_s)|} \frac{\Im E(\boldsymbol{P}_s)}{|E(\boldsymbol{P}_s)|}, \tag{B.12}$$

$$1 > \mp \Im \frac{(t-T)\left(1 - \boldsymbol{v}^2(\boldsymbol{P}_s)\right)}{\sigma E(\boldsymbol{P}_s)} = \pm \frac{t-T}{\sigma\, |E(\boldsymbol{P}_s)|} \frac{\left(1 - \Re \boldsymbol{v}^2(\boldsymbol{P}_s)\right) \Im E(\boldsymbol{P}_s) - \Re E(\boldsymbol{P}_s)\, \Im \boldsymbol{v}^2(\boldsymbol{P}_s)}{|E(\boldsymbol{P}_s)|}. \tag{B.13}$$

To summarize, the saddle-point method yields

$$\mathcal{U}_{s,\sigma;X,\boldsymbol{P}}(x) = \left(\frac{\sigma}{\pi}\right)^{3/4} \left(\frac{1}{2E_\Psi(\boldsymbol{P}_s)\,\sigma^3}\right)^{1/2} \frac{U(s,\boldsymbol{P}_s)\, e^{-iE_\Psi(\boldsymbol{P}_s)(t-T) + i\boldsymbol{P}_s\cdot(\boldsymbol{x}-\boldsymbol{X}) - \frac{\sigma}{2}(\boldsymbol{P}_s - \boldsymbol{P})^2}}{\left(1 \pm i\frac{t-T}{\sigma E_\Psi(\boldsymbol{P}_s)}\right)\sqrt{1 \pm i\frac{t-T}{\sigma E_\Psi(\boldsymbol{P}_s)}\left(1 - \boldsymbol{v}^2(\boldsymbol{P}_s)\right)}}, \tag{B.14}$$

$$\mathcal{V}_{s,\sigma;X,\boldsymbol{P}}(x) = \left(\frac{\sigma}{\pi}\right)^{3/4} \left(\frac{1}{2E_\Psi(\boldsymbol{P}_s)\,\sigma^3}\right)^{1/2} \frac{V(s,\boldsymbol{P}_s)\, e^{iE_\Psi(\boldsymbol{P}_s)(t-T) - i\boldsymbol{P}_s\cdot(\boldsymbol{x}-\boldsymbol{X}) - \frac{\sigma}{2}(\boldsymbol{P}_s - \boldsymbol{P})^2}}{\left(1 \pm i\frac{t-T}{\sigma E_\Psi(\boldsymbol{P}_s)}\right)\sqrt{1 \pm i\frac{t-T}{\sigma E_\Psi(\boldsymbol{P}_s)}\left(1 - \boldsymbol{v}^2(\boldsymbol{P}_s)\right)}}. \tag{B.15}$$

When necessary, we may expand them using

$$(E(\boldsymbol{P} + \Delta\boldsymbol{P}))^{-1/2} = \left(m^2 + (\boldsymbol{P} + \Delta\boldsymbol{P})^2\right)^{-1/4} = \left(m^2 + \boldsymbol{P}^2 + 2\boldsymbol{P}\cdot\Delta\boldsymbol{P} + \cdots\right)^{-1/4}$$
$$= (E(\boldsymbol{P}))^{-1/2}\left(1 - \frac{\boldsymbol{v}(\boldsymbol{P})\cdot\Delta\boldsymbol{P}}{2E(\boldsymbol{P})} + \cdots\right), \tag{B.16}$$

etc., and the leading-order result for the large-σ limit is[34]

$$\mathcal{U}_{s,\sigma;X,\boldsymbol{P}}(x) = \left(\frac{\sigma}{\pi}\right)^{3/4} \left(\frac{2\pi}{\sigma}\right)^{3/2} \left(\frac{1}{(2\pi)^3\, 2E_\Psi(\boldsymbol{P})}\right)^{1/2} U(s,\boldsymbol{P})\, e^{-iE_\Psi(\boldsymbol{P})(t-T) + i\boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{X}) - \frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t))^2}{2\sigma}}, \tag{B.17}$$

[33] Explicitly, one may, e.g., take

$$U = \begin{bmatrix} \frac{v_1 v_3}{\sqrt{v_1^2+v_2^2}\sqrt{\boldsymbol{v}^2}} & -\frac{v_2}{\sqrt{v_1^2+v_2^2}} & \frac{v_1}{\sqrt{\boldsymbol{v}^2}} \\ \frac{v_2 v_3}{\sqrt{v_1^2+v_2^2}\sqrt{\boldsymbol{v}^2}} & \frac{v_1}{\sqrt{v_1^2+v_2^2}} & \frac{v_2}{\sqrt{\boldsymbol{v}^2}} \\ -\frac{\sqrt{v_1^2+v_2^2}}{\sqrt{\boldsymbol{v}^2}} & 0 & \frac{v_3}{\sqrt{\boldsymbol{v}^2}} \end{bmatrix}.$$

[34] We have taken up to the σ^{-1} order in the exponent since the terms of order σ^0 are pure imaginary and just give a phase factor.

$$\mathcal{V}_{s,\sigma;X,\boldsymbol{P}}(x) = \left(\frac{\sigma}{\pi}\right)^{3/4} \left(\frac{2\pi}{\sigma}\right)^{3/2} \left(\frac{1}{(2\pi)^3\, 2E_\Psi(\boldsymbol{P})}\right)^{1/2} V(s,\boldsymbol{P})\, e^{iE_\Psi(\boldsymbol{P})(t-T)-i\boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{X})-\frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t))^2}{2\sigma}}. \tag{B.18}$$

This is used in Eqs. (18) and (115).

In the large-σ limit, we may iteratively solve the saddle-point condition of Eq. (B.6) by $\boldsymbol{P}_s = \boldsymbol{P} + \Delta_1\boldsymbol{P} + \Delta_2\boldsymbol{P} + \cdots$ with $\Delta_n\boldsymbol{P} = \mathcal{O}(\sigma^{-n})$. The result is

$$\boldsymbol{P}_s = \boldsymbol{P} \pm i\frac{\boldsymbol{x}-\boldsymbol{\Xi}(t)}{\sigma} + \mathcal{O}\left(\frac{1}{\sigma^2}\right), \tag{B.19}$$

where $\boldsymbol{\Xi}(t) := \boldsymbol{X} + \boldsymbol{V}(t-T)$ with $\boldsymbol{V} := \boldsymbol{v}(\boldsymbol{P})$, corresponding to Eq. (19). The zeroth and second derivatives read[35]

$$F_\pm(\boldsymbol{P}_s) = \mp iE(\boldsymbol{P})(t-T) \pm i\boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{X}) - \frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t))^2}{2\sigma} + \mathcal{O}\left(\frac{1}{\sigma^2}\right), \tag{B.20}$$

$$\frac{\partial^2 F_\pm(\boldsymbol{P}_s)}{\partial p_i \partial p_j} = -\sigma\delta_{ij} \mp i\frac{t-T}{E(\boldsymbol{P})}\left(\delta_{ij} - V_iV_j\right) + \mathcal{O}\left(\frac{1}{\sigma}\right), \tag{B.21}$$

where we used

$$E(\boldsymbol{P}_s) = E(\boldsymbol{P}) \pm i\frac{\boldsymbol{V}\cdot(\boldsymbol{x}-\boldsymbol{\Xi}(t))}{\sigma} + \mathcal{O}\left(\frac{1}{\sigma^2}\right), \tag{B.22}$$

$$\boldsymbol{v}(\boldsymbol{P}_s) = \boldsymbol{V} \pm i\frac{\boldsymbol{x}-\boldsymbol{\Xi}(t)-\boldsymbol{V}\left[\boldsymbol{V}\cdot(\boldsymbol{x}-\boldsymbol{\Xi}(t))\right]}{\sigma E(\boldsymbol{P})} + \mathcal{O}\left(\frac{1}{\sigma^2}\right). \tag{B.23}$$

In particular, the necessary conditions in Eqs. (B.12) and (B.13) read, at the leading order,

$$1 > \frac{t-T}{\sigma^2}\frac{\boldsymbol{V}\cdot(\boldsymbol{x}-\boldsymbol{\Xi}(t))}{\boldsymbol{P}^2+m^2}, \tag{B.24}$$

$$1 > -\frac{t-T}{\sigma^2}\frac{\boldsymbol{V}\cdot(\boldsymbol{x}-\boldsymbol{\Xi}(t))}{\boldsymbol{P}^2+m^2}\left(1-\boldsymbol{V}^2\right). \tag{B.25}$$

Appendix C. Wave and particle limits for decaying particle

C.1. Wave limit

In the wave limit of the initial state, $\sigma_0 \gg \sigma_a$, we get

$$\sigma_s \to \frac{\sigma_1\sigma_2}{\sigma_1+\sigma_2} =: \sigma_{\text{out}}, \tag{C.1}$$

and then Eqs. (42)–(45) reduce to

$$\Delta\boldsymbol{V}^2 \to \frac{\sigma_{\text{out}}}{\sigma_1+\sigma_2}\left(\boldsymbol{V}_1-\boldsymbol{V}_2\right)^2, \tag{C.2}$$

[35] We may also rewrite

$$\begin{aligned} F_\pm(\boldsymbol{P}_s) &= \mp i\frac{m^2}{E(\boldsymbol{P})}(t-T) \pm i\boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{\Xi}(t)) - \frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t))^2}{2\sigma} + \mathcal{O}\left(\frac{1}{\sigma^2}\right) \\ &= \mp i\frac{m^2}{E(\boldsymbol{P})}(t-T) - \frac{\sigma}{2}\boldsymbol{P}^2 - \frac{(\boldsymbol{x}-\boldsymbol{\Xi}(t)\mp i\sigma\boldsymbol{P})^2}{2\sigma} + \mathcal{O}\left(\frac{1}{\sigma^2}\right). \end{aligned}$$

$$\sigma_t \to \frac{\sigma_1+\sigma_2}{(\boldsymbol{V}_1-\boldsymbol{V}_2)^2}, \tag{C.3}$$

$$\mathfrak{T} \to -\frac{\sigma_1+\sigma_2}{\sigma_\text{out}}\left(\boldsymbol{V}_1-\boldsymbol{V}_2\right)\cdot\left(\boldsymbol{\mathfrak{X}}_1-\boldsymbol{\mathfrak{X}}_2\right), \tag{C.4}$$

$$\mathcal{R} \to \frac{(\boldsymbol{\mathfrak{X}}_1-\boldsymbol{\mathfrak{X}}_2)^2}{\sigma_1+\sigma_2}+\frac{\sigma_1+\sigma_2}{\sigma_\text{out}^2}\frac{[(\boldsymbol{V}_1-\boldsymbol{V}_2)\cdot(\boldsymbol{\mathfrak{X}}_1-\boldsymbol{\mathfrak{X}}_2)]^2}{(\boldsymbol{V}_1-\boldsymbol{V}_2)^2}, \tag{C.5}$$

where we used, for arbitrary $\boldsymbol{Q}_A$ and $\boldsymbol{Q}'_A$,

$$\overline{\boldsymbol{Q}\cdot\boldsymbol{Q}'}-\overline{\boldsymbol{Q}}\cdot\overline{\boldsymbol{Q}'} \to \frac{\sigma_\text{out}}{\sigma_1+\sigma_2}\left(\boldsymbol{Q}_1-\boldsymbol{Q}_2\right)\cdot\left(\boldsymbol{Q}'_1-\boldsymbol{Q}'_2\right). \tag{C.6}$$

(Recall that $\boldsymbol{\mathfrak{X}}_1-\boldsymbol{\mathfrak{X}}_2=\boldsymbol{X}_1-\boldsymbol{X}_2-\boldsymbol{V}_1T_1+\boldsymbol{V}_2T_2$.) Note that the $\boldsymbol{V}_0$ dependence drops out in the wave limit.[36]

In the limit, the eigenvalues in Eq. (93) become

$$\frac{2}{\sigma_1+\sigma_2}, \qquad \frac{1}{2\sigma_0}, \qquad \frac{1}{\sigma_0}\frac{(\boldsymbol{V}_1-\boldsymbol{V}_0)^2+(\boldsymbol{V}_2-\boldsymbol{V}_0)^2}{(\boldsymbol{V}_1-\boldsymbol{V}_2)^2}, \tag{C.7}$$

where the first two are each two-fold degenerate.

C.2. Particle limit

In the particle limit of the initial state $\sigma_0 \ll \sigma_a$, we obtain

$$\sigma_s \to \sigma_0, \tag{C.8}$$

$$\Delta\boldsymbol{V}^2 \to \sigma_0\left(\frac{(\delta\boldsymbol{V}_1)^2}{\sigma_1}+\frac{(\delta\boldsymbol{V}_2)^2}{\sigma_2}\right), \tag{C.9}$$

$$\sigma_t \to \left(\frac{(\delta\boldsymbol{V}_1)^2}{\sigma_1}+\frac{(\delta\boldsymbol{V}_2)^2}{\sigma_2}\right)^{-1}, \tag{C.10}$$

$$\mathfrak{T} \to -\frac{\frac{\delta\boldsymbol{\mathfrak{X}}_1\cdot\delta\boldsymbol{V}_1}{\sigma_1}+\frac{\delta\boldsymbol{\mathfrak{X}}_2\cdot\delta\boldsymbol{V}_2}{\sigma_2}}{\frac{(\delta\boldsymbol{V}_1)^2}{\sigma_1}+\frac{(\delta\boldsymbol{V}_2)^2}{\sigma_2}}, \tag{C.11}$$

$$\mathcal{R} \to \frac{(\delta\boldsymbol{\mathfrak{X}}_1)^2}{\sigma_1}+\frac{(\delta\boldsymbol{\mathfrak{X}}_2)^2}{\sigma_2}-\frac{\left(\frac{\delta\boldsymbol{\mathfrak{X}}_1\cdot\delta\boldsymbol{V}_1}{\sigma_1}+\frac{\delta\boldsymbol{\mathfrak{X}}_2\cdot\delta\boldsymbol{V}_2}{\sigma_2}\right)^2}{\frac{(\delta\boldsymbol{V}_1)^2}{\sigma_1}+\frac{(\delta\boldsymbol{V}_2)^2}{\sigma_2}}, \tag{C.12}$$

where we used, for arbitrary $\boldsymbol{Q}_A$ and $\boldsymbol{Q}'_A$,

$$\overline{\boldsymbol{Q}\cdot\boldsymbol{Q}'}-\overline{\boldsymbol{Q}}\cdot\overline{\boldsymbol{Q}'} \to \sigma_0\left(\frac{\delta\boldsymbol{Q}_1\cdot\delta\boldsymbol{Q}'_1}{\sigma_1}+\frac{\delta\boldsymbol{Q}_2\cdot\delta\boldsymbol{Q}'_2}{\sigma_2}\right). \tag{C.13}$$

(Recall that $\delta\boldsymbol{V}_a=\boldsymbol{V}_a-\boldsymbol{V}_0$ and that $\delta\boldsymbol{\mathfrak{X}}_a=\boldsymbol{X}_a-\boldsymbol{X}_0-T_a\boldsymbol{V}_a+T_0\boldsymbol{V}_0$.) The eigenvalues in Eq. (93) become

$$\frac{1}{\sigma_1}, \qquad \frac{1}{\sigma_2}, \qquad \frac{1}{\sigma_1\sigma_2}\frac{(\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2}{\frac{(\delta\boldsymbol{V}_1)^2}{\sigma_1}+\frac{(\delta\boldsymbol{V}_2)^2}{\sigma_2}}, \tag{C.14}$$

[36] Note, however, that the $\boldsymbol{V}_0$ dependence in the zero eigenvector in Eq. (91) still remains; see footnote 18.

where the first two are each two-fold degenerate.

More concretely,

$$\mathfrak{T} = -\frac{\frac{(\boldsymbol{X}_1-\boldsymbol{X}_0-\boldsymbol{V}_1T_1+\boldsymbol{V}_0T_0)\cdot(\boldsymbol{V}_1-\boldsymbol{V}_0)}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{X}_0-\boldsymbol{V}_2T_2+\boldsymbol{V}_0T_0)\cdot(\boldsymbol{V}_2-\boldsymbol{V}_0)}{\sigma_2}}{\frac{(\boldsymbol{V}_1-\boldsymbol{V}_0)^2}{\sigma_1}+\frac{(\boldsymbol{V}_2-\boldsymbol{V}_0)^2}{\sigma_2}}, \tag{C.15}$$

$$\mathcal{R} = \frac{(\boldsymbol{X}_1-\boldsymbol{X}_0-\boldsymbol{V}_1T_1+\boldsymbol{V}_0T_0)^2}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{X}_0-\boldsymbol{V}_2T_2+\boldsymbol{V}_0T_0)^2}{\sigma_2} - \frac{\left(\frac{(\boldsymbol{X}_1-\boldsymbol{X}_0-\boldsymbol{V}_1T_1+\boldsymbol{V}_0T_0)\cdot(\boldsymbol{V}_1-\boldsymbol{V}_0)}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{X}_0-\boldsymbol{V}_2T_2+\boldsymbol{V}_0T_0)\cdot(\boldsymbol{V}_2-\boldsymbol{V}_0)}{\sigma_2}\right)^2}{\frac{(\boldsymbol{V}_1-\boldsymbol{V}_0)^2}{\sigma_1}+\frac{(\boldsymbol{V}_2-\boldsymbol{V}_0)^2}{\sigma_2}}. \tag{C.16}$$

Without loss of generality, we may set $X_0 = (T_0, \boldsymbol{X}_0) = 0$, and then we obtain

$$\mathfrak{T} = -\frac{\frac{(\boldsymbol{X}_1-\boldsymbol{V}_1T_1)\cdot(\boldsymbol{V}_1-\boldsymbol{V}_0)}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{V}_2T_2)\cdot(\boldsymbol{V}_2-\boldsymbol{V}_0)}{\sigma_2}}{\frac{(\boldsymbol{V}_1-\boldsymbol{V}_0)^2}{\sigma_1}+\frac{(\boldsymbol{V}_2-\boldsymbol{V}_0)^2}{\sigma_2}}, \tag{C.17}$$

$$\mathcal{R} = \frac{(\boldsymbol{X}_1-\boldsymbol{V}_1T_1)^2}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{V}_2T_2)^2}{\sigma_2} - \frac{\left(\frac{(\boldsymbol{X}_1-\boldsymbol{V}_1T_1)\cdot(\boldsymbol{V}_1-\boldsymbol{V}_0)}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{V}_2T_2)\cdot(\boldsymbol{V}_2-\boldsymbol{V}_0)}{\sigma_2}\right)^2}{\frac{(\boldsymbol{V}_1-\boldsymbol{V}_0)^2}{\sigma_1}+\frac{(\boldsymbol{V}_2-\boldsymbol{V}_0)^2}{\sigma_2}}. \tag{C.18}$$

C.3. Decay at rest

Finally, we list the corresponding expression to Eqs. (42)–(45) for the decay at rest $\boldsymbol{V}_0 = 0$ (and hence $\boldsymbol{P}_0 = 0$ and $E_0 = m_0$), without taking any limit:

$$\Delta\boldsymbol{V}^2 = \sigma_s^2\left[\frac{\boldsymbol{V}_1^2}{\sigma_0\sigma_1}+\frac{\boldsymbol{V}_2^2}{\sigma_0\sigma_2}+\frac{(\boldsymbol{V}_1-\boldsymbol{V}_2)^2}{\sigma_1\sigma_2}\right], \tag{C.19}$$

$$\sigma_t = \frac{1}{\sigma_s}\left[\frac{\boldsymbol{V}_1^2}{\sigma_0\sigma_1}+\frac{\boldsymbol{V}_2^2}{\sigma_0\sigma_2}+\frac{(\boldsymbol{V}_1-\boldsymbol{V}_2)^2}{\sigma_1\sigma_2}\right]^{-1}, \tag{C.20}$$

$$\mathfrak{T} = -\frac{\frac{(\boldsymbol{X}_1-\boldsymbol{X}_0-\boldsymbol{V}_1T_1)\cdot\boldsymbol{V}_1}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{X}_0-\boldsymbol{V}_2T_2)\cdot\boldsymbol{V}_2}{\sigma_2}}{\frac{\boldsymbol{V}_1^2}{\sigma_1}+\frac{\boldsymbol{V}_2^2}{\sigma_2}}, \tag{C.21}$$

$$\mathcal{R} = \frac{(\boldsymbol{X}_1-\boldsymbol{X}_0-\boldsymbol{V}_1T_1)^2}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{X}_0-\boldsymbol{V}_2T_2)^2}{\sigma_2} - \frac{\left(\frac{(\boldsymbol{X}_1-\boldsymbol{X}_0-\boldsymbol{V}_1T_1)\cdot\boldsymbol{V}_1}{\sigma_1}+\frac{(\boldsymbol{X}_2-\boldsymbol{X}_0-\boldsymbol{V}_2T_2)\cdot\boldsymbol{V}_2}{\sigma_2}\right)^2}{\frac{\boldsymbol{V}_1^2}{\sigma_1}+\frac{\boldsymbol{V}_2^2}{\sigma_2}}. \tag{C.22}$$

An experimentalist-friendly parametrization for the decay at rest might be

$$(\delta\boldsymbol{P})^2 = p_1^2 + 2p_1p_2\cos\theta + p_2^2, \tag{C.23}$$

$$\delta\omega = E_1 + E_2 - m_0 - \frac{\sigma_s p_1}{\sigma_1 E_1}(p_1 + p_2\cos\theta) - \frac{\sigma_s p_2}{\sigma_2 E_2}(p_2 + p_1\cos\theta), \tag{C.24}$$

$$\sigma_t = \frac{\sigma_0\sigma_1\sigma_2}{\sigma_s}\frac{1}{(\sigma_0+\sigma_1)\frac{p_2^2}{E_2^2} - 2\sigma_0\frac{p_1p_2}{E_1E_2}\cos\theta + (\sigma_0+\sigma_2)\frac{p_1^2}{E_1^2}}, \tag{C.25}$$

where $p_a := |\boldsymbol{P}_a|$ for $a = 1, 2$; the angle is defined by $\cos\theta := \frac{\boldsymbol{P}_1\cdot\boldsymbol{P}_2}{p_1 p_2}$; and E_a and σ_s are given in Eqs. (28) and (30), respectively. One may further take the above plane-wave or particle limit to simplify the expression if one wishes.

Without loss of generality, we may set $X_0 = (T_0, \boldsymbol{X}_0) = 0$, and then Eqs. (C.21) and (C.22) further simplify to

$$\mathfrak{T} = -\frac{\frac{(\boldsymbol{X}_1-\boldsymbol{V}_1T_1)\cdot\boldsymbol{V}_1}{\sigma_1} + \frac{(\boldsymbol{X}_2-\boldsymbol{V}_2T_2)\cdot\boldsymbol{V}_2}{\sigma_2}}{\frac{\boldsymbol{V}_1^2}{\sigma_1} + \frac{\boldsymbol{V}_2^2}{\sigma_2}}, \tag{C.26}$$

$$\mathcal{R} = \frac{(\boldsymbol{X}_1 - \boldsymbol{V}_1T_1)^2}{\sigma_1} + \frac{(\boldsymbol{X}_2 - \boldsymbol{V}_2T_2)^2}{\sigma_2} - \frac{\left(\frac{(\boldsymbol{X}_1-\boldsymbol{V}_1T_1)\cdot\boldsymbol{V}_1}{\sigma_1} + \frac{(\boldsymbol{X}_2-\boldsymbol{V}_2T_2)\cdot\boldsymbol{V}_2}{\sigma_2}\right)^2}{\frac{\boldsymbol{V}_1^2}{\sigma_1} + \frac{\boldsymbol{V}_2^2}{\sigma_2}}. \tag{C.27}$$

To cultivate intuition, we present the results for a simple configuration $\sigma_2 = \sigma_1$, $\boldsymbol{V}_0 = 0$, $\boldsymbol{V}_2 = -\boldsymbol{V}_1$, and $T_1 = T_2 =: T_{\text{out}}$:

$$\mathfrak{T} = T_{\text{out}} - \frac{\boldsymbol{X}_1 - \boldsymbol{X}_2}{2\,|\boldsymbol{V}_1|} \cdot \frac{\boldsymbol{V}_1}{|\boldsymbol{V}_1|}, \tag{C.28}$$

$$\mathcal{R} = \frac{1}{\sigma_1}\left(\boldsymbol{X}_1^2 + \boldsymbol{X}_2^2 - \frac{1}{2}\left[\frac{\boldsymbol{V}_1}{|\boldsymbol{V}_1|}\cdot(\boldsymbol{X}_1 - \boldsymbol{X}_2)\right]^2\right). \tag{C.29}$$

Appendix D. Boundary contributions in the boundary limit

Here we present the boundary contributions in the boundary limit $|\mathfrak{T} - T_{\text{in/out}}| \ll \sqrt{\sigma_t}$, which might be applicable for $\sigma_t\,(\delta\omega)^2 \lesssim 1$ too.

As discussed in the paragraph containing Eq. (84), the expression in Eq. (106) is valid only when $\sigma_t\,(\delta\omega)^2 \gg 1$ at $\mathfrak{T} = T_{\text{in/out}}$. It might be convenient if we have an expression in the boundary limit $|\mathfrak{T} - T_{\text{in/out}}| \ll \sqrt{\sigma_t}$ valid for small $\delta\omega$ too. For that purpose, we expand the rational function in Eq. (83) around $\mathfrak{T} - T_{\text{in/out}} = 0$ and *naively* replace, by using Eq. (78), as

$$\frac{2}{\pi}\frac{1}{\sigma_t\,(\delta\omega)^2} \mapsto \left[\frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right) + e^{-\sigma_t(\delta\omega)^2}\right], \tag{D.1}$$

to obtain

$$e^{-\sigma_t(\delta\omega)^2}\,|G(\mathfrak{T})|^2 \simeq e^{-\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t}}\left[\frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right) + e^{-\sigma_t(\delta\omega)^2}\right]. \tag{D.2}$$

The first and second terms in the square brackets are exactly the dashed and dot-dashed lines, respectively, in Fig. 3 (and their sum is the solid line). For reference, we show the boundary contribution with this naive replacement:

$$dP \simeq \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\,2E_1}\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\,2E_2}(2\pi)^4\left(\sqrt{\frac{\sigma_t}{\pi}}\right)\left(\left(\frac{\sigma_s}{\pi}\right)^{3/2}e^{-\sigma_s(\delta\boldsymbol{P})^2}\right)$$
$$\times\sqrt{\frac{\sigma_t}{\pi^5}\left(\frac{\sigma_s}{\sigma_0\sigma_1\sigma_2}\right)^3}\,d^3\boldsymbol{X}_1\,d^3\boldsymbol{X}_2\,e^{-\mathcal{R}}e^{-\frac{(\mathfrak{T}-T_{\text{in/out}})^2}{\sigma_t}}\left[\frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right) + e^{-\sigma_t(\delta\omega)^2}\right]. \tag{D.3}$$

The formal limit, Eq. (107), of this expression reads

$$dP \to \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\,2E_1}\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\,2E_2}(2\pi)^4\left(\sqrt{\frac{\sigma_t}{\pi}}\right)\left(\left(\frac{\sigma_s}{\pi}\right)^{3/2}e^{-\sigma_s(\delta\boldsymbol{P})^2}\right)$$
$$\times\sqrt{\frac{\sigma_t}{\pi^5}\left(\frac{\sigma_s}{\sigma_0\sigma_1\sigma_2}\right)^3}\,d^6y\,e^{-\mathcal{R}}\sqrt{\pi\sigma_t}\,\delta(\mathfrak{T}-T_{\text{in/out}})\left[\frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right)+e^{-\sigma_t(\delta\omega)^2}\right]. \quad \text{(D.4)}$$

Naively, integration over $d^5y\,e^{-\mathcal{R}}$ would again give Eq. (99), and then the y_0 integral over the delta function gives the extra factor $\sqrt{(\delta\boldsymbol{V}_1)^2+(\delta\boldsymbol{V}_2)^2}$:

$$dP = \frac{\kappa^2}{2}\frac{1}{2E_0}\frac{d^3\boldsymbol{P}_1}{(2\pi)^3\,2E_1}\frac{d^3\boldsymbol{P}_2}{(2\pi)^3\,2E_2}(2\pi)^4\left(\left(\frac{\sigma_s}{\pi}\right)^{3/2}e^{-\sigma_s(\delta\boldsymbol{P})^2}\right)\sigma_t\left[\frac{4}{\pi}F^2\left(\sqrt{\frac{\sigma_t}{2}}\delta\omega\right)+e^{-\sigma_t(\delta\omega)^2}\right]. \quad \text{(D.5)}$$

Recall that $\delta\boldsymbol{P}$, $\delta\omega$, and σ_t simplify to Eqs. (C.23)–(C.25) for the case of the decay at rest.

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