Graviton particle statistics from classical scattering amplitudes

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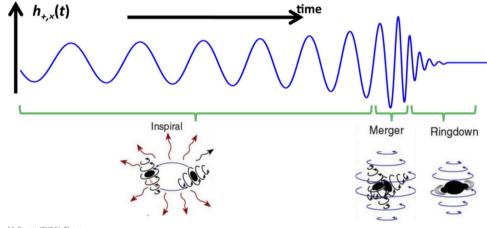
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<u>Mergers of binary black holes produce</u> <u>detectable gravitational waves</u>



M. Favata/SXS/K. Thorne

Detailed prediction of waveform needed for precision studies and tests of new physics. Techniques from amplitudes can help in the inspiral phase.

Classical gravitational observables from amplitudes

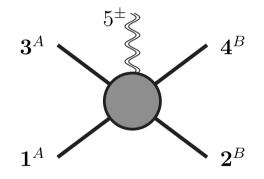
- Classical observables are analytically continued from bound orbits to hyperbolic scattering orbits. [Kälin, Porto]
- Scatter two wavepackets with impact parameter b^{μ} and measure the change in an observable O. [Kosower, Maybee, O'Connell]

$$\Delta \mathcal{O} = \langle \mathsf{out} \, | \, \mathcal{O} \, | \, \mathsf{out} \rangle - \langle \mathsf{in} \, | \, \mathcal{O} \, | \, \mathsf{in} \rangle$$

• S-matrix relations: $|\operatorname{out}\rangle = S |\operatorname{in}\rangle$, S = 1 + iT.

Gravitational radiation

- Massless particles aren't localized
- Classical wave in a pure state ~ coherent state
- Coherence characterizes statistics of emitted particles: Poisson distribution



- For the two-body problem, we consider particle statistics of emitted gravitons and examine deviations from Poisson distribution.
- Aim: identify amplitudes that do/don't contribute to the classical limit.
- Related work motivates the close study of 2-graviton emission at tree level. [Luna, Nicholson, O'Connell, White; Cristofoli, Gonzo, Moynihan, O'Connell, Ross, Sergola, White]
- Amplitudes computed from a Lagrangian with an auxiliary field
- On-shell recursion gives compact expressions, better suited for analysis of the classical limit.

Classical observables: the KMOC formalism

[Kosower, Maybee, O'Connell]

$$|\psi_{\text{in}}\rangle = \int d\Phi(p_1, p_2) \, e^{i \mathbf{b} \cdot p_1/\hbar} \, \psi_A(p_1) \psi_B(p_2) \, |p_1 p_2\rangle,$$

where
$$d\Phi(p) = d^4p \,\delta(p^2 - m^2) \,\theta(p^0)$$
,

and
$$\psi(p) \sim m^{-1} \exp\left[-\frac{p \cdot v}{\hbar \ell_c / \ell_w^2}\right]$$
.

Separation of scales for classical scattering: $\ell_c \ll \ell_w \ll b$.

Massive particles localized on classical trajectories as $\hbar \to 0$.

Coherent states for gravitons

[Cristofoli, Gonzo, Kosower, O'Connell]

- Massless particles (e.g. gravitons) cannot be localized; single gravitons are not classical.
- Every quantum state of radiation (or density matrix) is a superposition of coherent states. [Glauber]
- But our in state $|\psi_{in}\rangle$ is pure, and the S matrix is unitary, so the out state is a pure state. Thus it must be a single coherent state in the classical limit $\hbar \rightarrow 0$.
- Coherent state for a graviton of momentum k and helicity σ : $|\alpha_k^{\sigma}\rangle = \exp\left[\alpha_k a_{\sigma}^{\dagger}(k) - \alpha_k^* a_{\sigma}(k)\right]|0\rangle$ [Glauber-Suradashan]
- Promote to infinite superposition of momenta: $|\alpha^{\sigma}\rangle = \exp\left[\int d\Phi(k)(\alpha(k)a_{\sigma}^{\dagger}(k) - \alpha^{*}(k)a_{\sigma}(k))\right]|0\rangle$

Coherence and the Poisson distribution

Coherent state expanded in graviton-number states:

$$|\alpha^{\sigma}\rangle = \exp\left(-\frac{1}{2}\int d\Phi(k) |\alpha^{\sigma}(k)|^{2}\right) \sum_{n=0}^{\infty} \frac{1}{n!} \int \prod_{i=1}^{n} \left[d\Phi(k_{i})\alpha^{\sigma}(k_{i})\right] |k_{1}^{\sigma} \dots k_{n}^{\sigma}\rangle$$

Probability of detecting *n* gravitons with helicity σ' :

$$P_n^{\sigma'} = \delta_{\sigma\sigma'} \exp\left(-\int d\Phi(k) \left| \alpha^{\sigma}(k) \right|^2\right) \frac{1}{n!} \left(\int d\Phi(k) \left| \alpha^{\sigma}(k) \right|^2\right)^n$$

Poisson statistics are equivalent to coherence of the state.

Counting emitted gravitons

[cf. Gelis, Venugopalan in QCD]

Probability of emitting *n* gravitons:

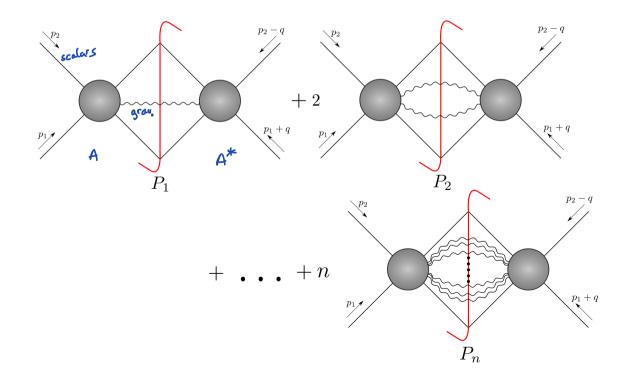
$$\bar{P}_{n} = \frac{1}{n!} \sum_{\sigma_{1},\dots,\sigma_{n}=\pm} \int d\Phi(p_{3}) d\Phi(p_{4}) \int d\Phi(k) \left| \left\langle k_{1}^{\sigma_{1}}\dots k_{n}^{\sigma_{n}} p_{3} p_{4} \right| S \left| p_{1} p_{2} \right\rangle \right|^{2}$$

with an implicit IR cutoff.

Unitarity:
$$\sum_{n=0}^{\infty} \bar{P}_n = 1.$$

Graviton number operator

 $\hat{N} = \sum_{\sigma=\pm} \int d\Phi(k) \, a_{\sigma}^{\dagger}(k) a_{\sigma}(k). \qquad \text{Mean: } \mu_{\text{out}} = \langle \psi_{\text{out}} \, | \, \hat{N} \, | \, \psi_{\text{out}} \rangle = \sum_{n=0}^{\infty} n \, P_n.$



Graviton particle statistics

• Mean:
$$\mu_{\text{out}} = \langle \psi_{\text{out}} | \hat{N} | \psi_{\text{out}} \rangle = \sum_{n=0}^{\infty} n P_n$$

• Variance:

$$\Sigma_{\text{out}} = \langle \psi_{\text{out}} | (\hat{N})^2 | \psi_{\text{out}} \rangle - \left(\langle \psi_{\text{out}} | \hat{N} | \psi_{\text{out}} \rangle \right)^2 = \sum_{n=0}^{\infty} n^2 P_n - \left(\sum_{n=0}^{\infty} n P_n \right)^2$$

2

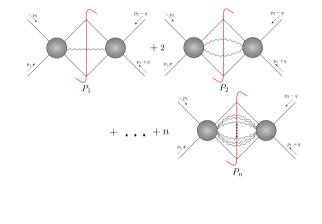
• In a Poisson distribution, Mean=Variance. Hence we define $\Delta_{out} = \Sigma_{out} - \mu_{out}$ and check whether this deviation vanishes. Also check higher moments.

Graviton particle statistics

Expand in powers of the gravitational coupling G.

$$P_{n} = \sum_{L_{1},L_{2}} G^{2+n+L_{1}+L_{2}} P_{n}^{(L_{1},L_{2})}$$

Leading order: $\Delta_{\text{out}} \Big|_{\mathcal{O}(G^{4})} = 2G^{4} P_{2}^{(0,0)}.$



Product of 6-point tree amplitudes. Do these amplitudes survive in the classical limit?

For the classical limit, we will examine \hbar scaling and check whether $\hbar \Delta_{out} \rightarrow 0$.

Computing amplitudes

- The Einstein-Hilbert action suffers from a proliferation of vertices with gauge dependence.
- With an auxiliary field and explicit gauge fixing, a compact form of the tree-level Lagrangian is obtained with only cubic interactions.
- We add minimally coupled scalars for the massive particles.

$$S_{\rm GR} = \frac{1}{16\pi G} \int d^4x \left[-\left(A^a_{bc}A^b_{ad} - \frac{1}{3}A^a_{ac}A^b_{bd}\right)\sigma^{cd} + A^a_{bc}\partial_a\sigma^{bc} \right]$$

where
$$\sigma^{ab} = \sqrt{-g} g^{ab}$$
;

$$S_{\text{matter}} = -\sum_{\substack{j=A,B\\\text{two scalars}}} \int d^4x \left[\frac{1}{2} \sigma^{ab} \partial_a \phi_j \partial_b \phi_j + \frac{1}{2} \sqrt{-\det(\sigma^{-1})} m_j^2 \phi_j^2 \right]$$

$$\mathscr{L}_{\text{GF}} = -\frac{1}{2} \eta_{cd} \partial_a \left(\sqrt{-g} g^{ac} \right) \partial_b \left(\sqrt{-g} g^{bd} \right)$$

With the massive scalars, interaction vertices do proliferate beyond cubic ones, but are under control at lower orders.

Interactions through order h^3 : *hhh*, *hhA*, *hAA*, *h\phi\phi*, *hh\phi\phi*, *hhh\phi\phi*.

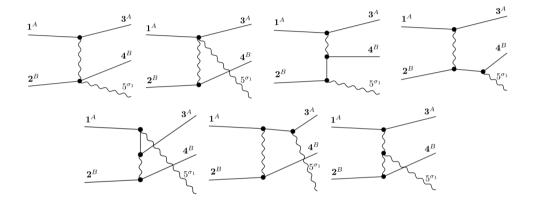
$\underbrace{\begin{array}{c} 4-\text{point amplitude} \\ \underline{1^{A}} & \underline{3^{A}} \\ \underline{2^{B}} & \underline{4^{B}} \end{array}}_{2^{B}}$

- n = 0. No graviton emission.
- Irrelevant for mean, variance, etc.; ingredient for recursive constructions.
- Single Feynman diagram

 $K = \sqrt{32\pi G}$

$$\mathscr{A}_{4}^{(0)}(\mathbf{1}^{A},\mathbf{2}^{B},\mathbf{3}^{A},\mathbf{4}^{B}) = -\frac{i\kappa^{2}}{2t}\left(\frac{1}{2}t\left(-m_{A}^{2}-m_{B}^{2}+s\right) + \frac{1}{2}\left(-m_{A}^{2}-m_{B}^{2}+s\right)^{2} - m_{A}^{2}m_{B}^{2}\right)$$

5-point amplitude



- 7 Feynman diagrams
- Prefer a compact formula, but with only one massless particle, there is no BCFW shift
- Introduce a new equal-mass shift

BCFW Recursion

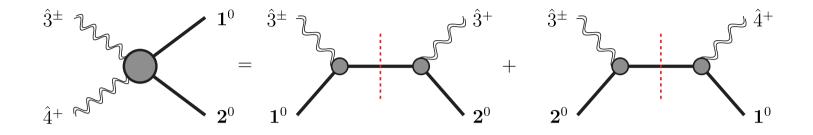
[RB, Cachazo, Feng, Witten]

- Consider a tree-level amplitude as a function of momenta, $\mathscr{A}_n(\{p_i\})$. Introduce a complex variable *z* through a momentum shift, $\hat{p}_i = p_i + zr_i$.
- If momentum is conserved, $\Sigma_i r_i = 0$, and momenta stay on shell, $\hat{p}_i^2 = m_i^2$, then the shifted function $\mathscr{A}_n(\{\hat{p}_i\})$ maintains properties of an amplitude.
- Further, if all $r_i \cdot r_j = 0$, then propagators depend linearly on z, so $\mathscr{A}_n(\{\hat{p}_i\})$ has only simple poles. If the residue at infinity (boundary term) vanishes, then we can apply Cauchy's residue theorem.

BCFW Recursion

•
$$\oint_{\gamma_{\infty}} dz \frac{\mathscr{A}_n(z)}{z} = \mathscr{A}_n(0) + \sum_I \operatorname{Res}_{z=z_I} \left[\frac{\mathscr{A}_n(z)}{z} \right]$$

•
$$\sum_{I} \operatorname{Res}_{z=z_{I}} \left[\frac{\mathscr{A}_{n}(z)}{z} \right] = -\sum_{I} \sum_{\sigma=\pm} \mathscr{A}_{L} \left(\{ \hat{p}_{L} \}, \hat{P}_{I}^{\sigma} \right) \frac{i}{P_{I}^{2} - m_{I}^{2}} \mathscr{A}_{R} \left(-\hat{P}_{I}^{-\sigma}, \{ \hat{p}_{R} \} \right)$$



Convenient momentum shift with spinor variables:

$$\hat{p}_{3}^{a\dot{b}} = |3\rangle^{a} [\hat{3}|^{\dot{b}} = |3\rangle^{a} ([3|+z[4|)^{\dot{b}},$$
$$\hat{p}_{4}^{a\dot{b}} = |\hat{4}\rangle^{a} [4|^{\dot{b}} = (|4\rangle - z|3\rangle)^{a} [4|^{\dot{b}}.$$

Result:

$$\mathscr{A}_{4}^{(0)}(\mathbf{1}^{A}, \mathbf{2}^{A}, 3^{+}, 4^{+}) = -i\kappa^{2} \frac{m_{A}^{4}[34]^{3}}{\langle 34 \rangle (s_{31} - m_{A}^{2})(s_{32} - m_{A}^{2})},$$
$$\mathscr{A}_{4}^{(0)}(\mathbf{1}^{A}, \mathbf{2}^{A}, 3^{-}, 4^{+}) = i\kappa^{2} \frac{[4 | 1 | 3 \rangle^{4}}{s_{34}(s_{31} - m_{A}^{2})(s_{32} - m_{A}^{2})}.$$

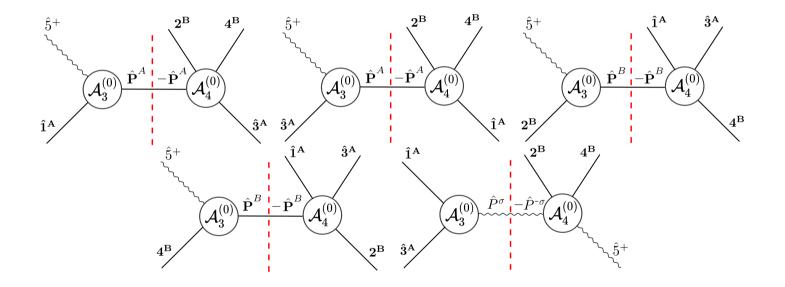
The equal-mass shift

- Since the masses are just parameters in the procedure, we can relax the on-shell condition: $\hat{p}_i^2 = \hat{m}_i^2$. Nonzero masses can vary, provided that any equal masses remain equal in the shift.
- For our 5-point amplitude, use $\hat{p}_5 = |\hat{5}\rangle[\hat{5}| = (|5\rangle + z (1 - 3)|5])[5|$ $\hat{p}_1 = p_1 + z |5][5|$ $\hat{p}_3 = p_3 - z |5][5|$

•
$$\hat{p}_1^2 = p_1^2 - z[5|13|5] = m_A^2 + z[5|31|5] = \hat{p}_3^2$$
.

• Vanishing of boundary term is hard to prove. We checked it with FD.

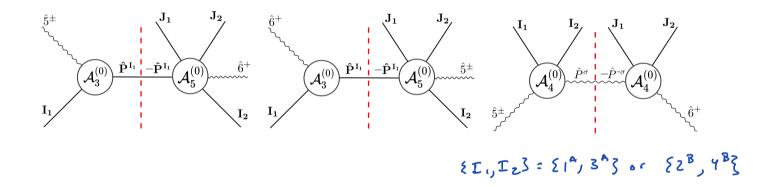
5-point factorization diagrams



5-point result

$$\begin{split} \mathcal{A}_{5}^{(0)} \left(\mathbf{1}^{A}, \mathbf{2}^{B}, \mathbf{3}^{A}, \mathbf{4}^{B}, 5^{+}\right) &= \frac{i\kappa^{3}}{8} \left(\left[\frac{-p_{4} \cdot p_{2}[5|13|5]^{2}}{s_{24}(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})} + \frac{[5|K_{A}K_{B}|5]^{2} - 8[5|13|5]^{2}}{16s_{13}s_{24}} \right. \\ &+ \frac{(m_{A}^{2} + m_{B}^{2})[5|13|5](2(s_{13} - s_{24})[5|13|5] + [5|K_{B}|5\rangle[5|K_{A}K_{B}|5])}{8(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &- \frac{K_{A} \cdot K_{B}(s_{24} - s_{13})^{2}[5|13|5](4s_{24}[5|42|5] - [5|K_{A}|5\rangle[5|K_{A}K_{B}|5])}{32s_{13}s_{24}(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &- \frac{K_{A} \cdot K_{B}[5|42|5]([5|K_{B}|5\rangle[5|K_{A}K_{B}|5] - 4(s_{13} + s_{24})[5|13|5])}{8s_{13}s_{24}(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &- \frac{K_{A} \cdot K_{B}[5|K_{A}|5\rangle[5|K_{B}|5\rangle([5|K_{A}K_{B}|5]^{2} - 8[5|42|5]^{2})}{8s_{13}s_{24}(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &- \frac{K_{A} \cdot K_{B}[5|K_{A}|5\rangle[5|K_{B}|5\rangle([5|K_{A}K_{B}|5]^{2} - 8[5|42|5]^{2})}{8s_{13}s_{24}(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &+ (\operatorname{tr}(K_{A}K_{B}K_{A}K_{B}) + 2[5|K_{A}|5\rangle^{2} + 2[5|K_{B}|5\rangle^{2} - 2s_{13}^{2} - 2s_{24}^{2}) \\ \times \left(\frac{[5|K_{A}|5\rangle[5|K_{B}|5\rangle[5|K_{B}|5\rangle[5|13|5][5|42|5]}{64s_{13}s_{24}(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &+ \frac{[5|42|5](2(s_{13} - s_{24})[5|42|5] - [5|K_{A}|5\rangle[5|K_{A}K_{B}|5])}{64s_{13}(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &+ \frac{[5|42|5](2(s_{13} - s_{24})[5|42|5] - [5|K_{A}|5\rangle[5|K_{A}K_{B}|5])}{64s_{13}(s_{51} - m_{A}^{2})(s_{53} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \\ &+ \frac{[5|42|5](2(s_{13} - s_{24})[5|42|5] - [5|K_{A}|5\rangle[5|K_{A}K_{B}|5])}{64s_{13}(s_{51} - m_{A}^{2})(s_{52} - m_{B}^{2})(s_{54} - m_{B}^{2})} \right] + [(1, 3, K_{A}) \leftrightarrow (2, 4, K_{B})] \right).$$

The 6-point amplitude

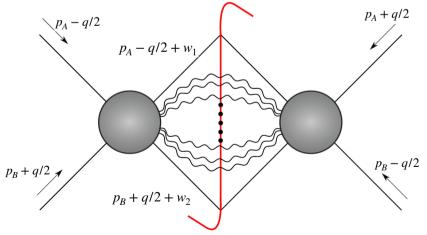


Usual BCFW shift on graviton pair.

Vanishing of boundary term verified from FD.

The classical limit

- KMOC told us how to set up the states. They also provide a detailed prescription for taking the classical limit. [Kosower, Maybee, O'Connell]
- Study how all quantities scale with \hbar , then take the limit $\hbar \to 0$.



- Momentum transfers q_j, w_j
 - Wavenumbers

$$\bar{q} = q/\hbar, \ \bar{w}_j = w_j/\hbar, \ \bar{k}_i = k_i/\hbar$$

• Coupling
$$\kappa \to \kappa / \sqrt{\hbar}$$

Classical limit of the tree amplitudes

• Implement explicit scaling: $\bar{q} = q/\hbar$, $\bar{w}_j = w_j/\hbar$, $\bar{k}_i = k_i/\hbar$, $\kappa \to \kappa/\sqrt{\hbar}$

• Replace velocities on classical trajectories: $p_j = \tilde{m}_j v_j$, $\tilde{m}_j^2 = m_j^2 - \hbar^2 \frac{\bar{q}^2}{4}$

• Naively expected behavior from Feynman diagrams: $\mathscr{A}_{5} = C_{1}^{(5)}\hbar^{-\frac{9}{2}} + C_{2}^{(5)}\hbar^{-\frac{7}{2}} + \mathscr{O}\left(\hbar^{-\frac{5}{2}}\right),$ $\mathscr{A}_{6} = C_{1}^{(6)}\hbar^{-6} + C_{2}^{(6)}\hbar^{-5} + C_{3}^{(6)}\hbar^{-4} + \mathscr{O}\left(\hbar^{-3}\right).$

Leading orders are suppressed:
$$\begin{aligned} C_1^{(5)} &= 0, \qquad C_2^{(5)} \neq 0, \\ C_1^{(6)} &= C_2^{(6)} = 0, \qquad C_3^{(6)} \neq 0. \end{aligned}$$

Classical limit of the 5-point amplitude

•
$$n = 1$$
, and $\mathscr{A}_5 = C_2^{(5)}\hbar^{-\frac{7}{2}} + \mathcal{O}\left(\hbar^{-\frac{5}{2}}\right)$.

- Leading order matches a known result. [Luna, Nicholson, O'Connell, White]
- The scaling of the *energy* of emitted radiation must remain finite, so the leading-order scaling for a contribution to the classical limit is compensated by precisely $\hbar^{5/2+n}$ for each amplitude.
- Probabilities should be treated as $\hbar P_n$.
- The 5-point tree does give a classical contribution: $\lim_{\hbar \to 0} \hbar P_1^{(0,0)} \sim \mathcal{O}(1)$.

Classical limit of the 6-point amplitude

•
$$n = 2$$
, and $\mathscr{A}_6 = C_3^{(6)}\hbar^{-4} + \mathcal{O}(\hbar^{-3}).$

- No classical contribution: $\lim_{\hbar \to 0} \hbar P_2^{(0,0)} = 0.$
- Leading order is new, and provides the first check of coherence. $\lim_{\hbar \to 0} \hbar \Delta_{\text{out}} \bigg|_{\mathcal{O}(G^4)} = 0.$

Coherence at higher orders

- At tree-level, we see the origin of \hbar suppression from the BCFW shift, so we conjecture: $\lim_{\hbar \to 0} \mathscr{A}_{4+n} \sim \hbar^{-3-\frac{n}{2}}$. Hence only the 5-point amplitude provides a classical contribution.
- . Conjecturally then, $\lim_{\hbar \to 0} \hbar P_n^{(0,0)} = 0$ for n > 2.
- Consistent with expectations of coherence. If coherence holds to higher orders in G and L, then there must be further relations among amplitudes, in the classical limit.

Coherence at higher orders

- Higher (factorial) moments: $\Gamma^{(m)} = \langle \psi | \hat{N}(\hat{N}-1)...(\hat{N}-m+1) | \psi \rangle$.
- For a Poisson distribution, $\Gamma^{(m)} = \mu^m$.
- Thus we check the vanishing of $\Delta^{(m)} = \Gamma^{(m)} \mu^m$. We have already done m = 2.

$$\Delta^{(m)} = \sum_{n} \sum_{L_{1},L_{2}} G^{2+n+L_{1}+L_{2}} \frac{n!}{(n-m)!} P_{n}^{(L_{1},L_{2})}$$
$$- \sum_{n_{1},\dots,n_{m}} \sum_{L_{1}^{(1)},\dots,L_{1}^{(m)}} \sum_{L_{2}^{(1)},\dots,L_{2}^{(m)}} G^{2m+\sum_{k} \left[n_{k}+L_{1}^{(k)}+L_{2}^{(k)}\right]} \prod_{j} \left[n_{j} P_{n_{j}}^{\left(L_{1}^{(j)},L_{2}^{(j)}\right)}\right]$$

Relations among amplitudes

$$\begin{split} & \text{Up to } \mathcal{O}(G^7), \\ & \lim_{\hbar \to 0} \hbar \Delta^{(2)} = \lim_{\hbar \to 0} \hbar \left(G^6 (2P_2^{(2,0)} + 2P_2^{(0,2)}) \right) \\ & \quad + \lim_{\hbar \to 0} \hbar \left(G^7 (2P_2^{(3,0)} + 2P_2^{(0,3)} + 6P_3^{(2,0)} + 6P_3^{(0,2)} + 6P_3^{(1,1)}) \right) \\ & \quad + \lim_{\hbar \to 0} \hbar \left[G^6 (2P_2^{(1,1)} - (P_1^{(0,0)})^2) + G^7 (2P_2^{(1,2)} + 2P_2^{(2,1)} - 2P_1^{(0,1)}P_1^{(0,0)} - 2P_1^{(1,0)}P_1^{(0,0)}) \right], \\ & \quad \lim_{\hbar \to 0} \hbar \Delta^{(3)} = \lim_{\hbar \to 0} \hbar \left(G^7 (6P_3^{(0,2)} + 6P_3^{(2,0)} + 6P_3^{(1,1)}) \right) \end{split}$$

Thus, coherence implies $\lim_{\hbar \to 0} \hbar \left(G^7 (6P_3^{(0,2)} + 6P_3^{(2,0)} + 6P_3^{(1,1)}) \right) = 0.$

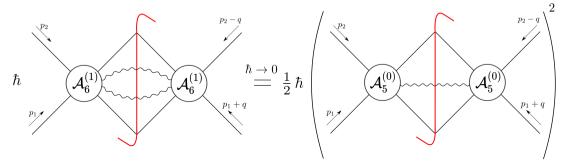
We make one more assumption, $\lim_{\hbar \to 0} \hbar P_n^{(L,0)} = \lim_{\hbar \to 0} \hbar P_n^{(0,L)} = 0$ for $n \ge 2$. [cf. Cristofoli, Gonzo, Moynihan, O'Connell, Ross, Sergola, White]

Relations among amplitudes

• $\lim_{\hbar \to 0} \hbar P_3^{(1,1)} = 0$: the 7-point 1-loop amplitude is classically suppressed.

$$\begin{split} \hbar P_2^{(1,1)} &= \frac{1}{2} \hbar (P_1^{(0,0)})^2 \\ \bullet \ \hbar (P_2^{(1,2)} + P_2^{(2,1)}) &= \hbar (P_1^{(0,1)} P_1^{(0,0)} + P_1^{(1,0)} P_1^{(0,0)}) \end{split} \text{ as } \hbar \to 0 \text{:} \end{split}$$

6- and higher-point amplitudes are related to 5-point at lower loop level.



Summary & Outlook

- "Amplitudes" techniques have been useful for precision calculations in the study of gravitational waves.
- Main result: classical suppression of a 6-pt tree amplitude as $\hbar \to 0$. Evidence for coherence of final semiclassical radiation state in binary scattering.
- Introduced an equal-mass shift for on-shell recursion.
- Conjectured higher-order relations in this framework, such that the 4- and 5-point amplitudes encode all information of the final state.
- Future directions:
 - explore higher-order relations, and connections to classical soft theorems
 - nonperturbative effects may spoil coherence
 - spin/tidal effects may spoil coherence
 - · resummation of radiation reaction effects is desirable