Light-front Schrödinger wave equation

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November 29, 2021

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Discussion on August 4, 2021

General discussions

- Recent reads, thoughts, plans and other things
- English, physics
- Literatures in HEP (search engine, Wikipedia, arXiv, inspirehep, indico)

Light-front Schrödinger wave equation

LFSWE provides a semiclassical first approximation to QCD

$$\Big[\frac{\vec{k}_\perp^2+m_q^2}{x}+\frac{\vec{k}_\perp^2+m_{\bar{q}}^2}{1-x}+V\Big]\psi_{s\bar{s}/h}(x,\vec{k}_\perp)=M_h^2\psi_{s\bar{s}/h}(x,\vec{k}_\perp)$$

- Separation of variables $V=V_\perp+V_\parallel$, $\psi=\phi(\zeta_\perp)\chi(x)$, $M^2=M_\perp^2+M_\parallel^2$

$$[\nabla_{\zeta\perp}^2+V_\perp]\phi(\vec{\zeta}_\perp)=M_\perp^2\phi(\vec{\zeta}_\perp)$$
$$\Big[\frac{m_q^2}{x}+\frac{m_{\bar{q}}^2}{1-x}+V_\parallel\Big]\chi(x)=M_\parallel^2\chi(x)$$

- Light-front holography, confinement and supersymmetry
- 't Hooft model, chiral symmetry breaking and longitudinal dynamics

Numerical methods

Goal: Develop numerical tools to solve LFSWEs.

1. Non-relativistic Schrödinger equations

Problem 1.1: Consider a 1D square well defined by the potential energy,

$$V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & x < 0 \text{ or } x > a. \end{cases} \tag{1}$$

A non-relativistic particle with mass m is inside the well. Find the energy levels of the particle and the corresponding wave functions.

Problem 1.2: In 1935, Hideki Yukawa proposed a meson-mediated model for nuclear force. In this model, two nucleon interacts by exchange a pion. Deuteron is a nucleus consisting of two nucleon. In the semiclassical approximation, it can be described by the 3D Schrödinger equation with Yukawa potential,

$$\left[\frac{\vec{p}^2}{2m_r} - \alpha\frac{\exp(-\mu r)}{r}\right]\psi(\vec{r}) = E\psi(\vec{r}). \tag{2}$$

Solve this equation and obtain the binding energies as well as the wave functions.

Numerical methods

Goal: Develop numerical tools to solve LFSWEs.

2. Light-front Schrödinger wave equations

Problem 2.1: Consider a 1D light-front Schrödinger equations,

$$\Big[\frac{m_q^2}{x(1-x)} - \sigma^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}\Big]\chi(x) = M^2\chi(x) \tag{3}$$

This equation describes a semiclassical model of the meson. m_q is the mass of the quark, $x = p_q^+ / P_M^+$ is the fraction of the quark momentum with respect to the meson of the meson. $\sigma \sim 1\,\mathrm{GeV}$ is the strength of the confining potential. Find the squared mass eigenvalues of the meson M^2 and the corresponding wavefunctions χ.

Problem 2.2: 't Hooft model is obtained from the 1D QCD at large N_c limit ['t Hooft, 1974 Nucl. Phys. B]. The equation is,

$$\Big[\frac{m_q^2}{x} + \frac{m_{\bar{q}}^2}{1-x}\Big]\chi(x) + \frac{g^2}{\pi}\mathrm{P}\int \mathrm{d}x' \frac{\chi(x)-\chi(x')}{(x-x')^2} = M^2\chi(x) \tag{4}$$

g is the dimensionful 't Hooft coupling. $\mathrm{P}\int$ means that the integral is taken with the principal value prescription.

Discussion on August 13, 2021

General discussions

- Thoughts sharing

Time-independent Schrödinger wave equation

$$H|\psi_h\rangle = E_h|\psi_h\rangle$$

Here $H = T + V$ is the Hamiltonian operator. T is kinetic energy, V is potential energy.

Representations:

$$\begin{aligned}|\psi\rangle &= \int \mathrm{d}^3x\, \psi(\vec{x})|\vec{x}\rangle, \\ &= \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, \psi(\vec{p})|\vec{p}\rangle\end{aligned}$$

$\psi(\vec{x})$ and $\psi(\vec{p})$ are called the coordinate space and momentum space wave functions, respectively. They are related by Fourier transform.

$$\psi(\vec{p}) = \int \mathrm{d}^3x\, e^{-i\vec{p}\cdot\vec{x}}\psi(\vec{x}).$$

Inner product:

$$\langle\psi|\varphi\rangle = \int \mathrm{d}^3x\, \psi(\vec{x})\varphi^*(\vec{x}) = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, \psi(\vec{p})\varphi^*(\vec{p})$$

Numerical methods

- Separation of variables, symmetry
- Finite difference (P1.1, P1.2, P2.1)
- Basis expansion
  - Fourier transform/plane wave basis (P1.1, P2.1)
  - Harmonic oscillator basis, Coulomb basis
- Nystrøm method (P1.2, P2.2)

Each method has its advantages and disadvantages in a specific set of problems.

Finite difference

$$\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \Big) \psi(x) = E\psi(x). \quad (a < x < b)$$

- Represent wave function on a set of finite discrete spatial points: $\{a = x_0, x_1, x_2, \cdots, x_{N-1}, x_N = b\}$
- Approximate the kinetic energy operator using finite difference,

$$\frac{\mathrm{d}}{\mathrm{d}x}\psi(x_i) = \frac{\psi_{i+1} - \psi_{i-1}}{2\Delta x} + O(\Delta x^2),$$
$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x_i) = \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{\Delta x^2} + O(\Delta x)$$

  where, $\Delta x = (b-a)/N$, $\psi_i \equiv \psi(x_i)$. The equation becomes ($V_i \equiv V(x_i)$),

$$2\psi_i - \psi_{i+1} - \psi_{i-1} + \Delta x^2 V_i \psi_i = E\Delta x^2 \psi_i,$$

- Solve the finite-discretized Schrödinger equation using eigensolvers

$$\sum_j H_{ij}\psi_j = \epsilon\psi_i,$$

  where $H_{ij} = \delta_{ij}(2 + \Delta x^2 V_i) - \delta_{j,i+1} - \delta_{i,j+1}$, $\epsilon = E\Delta x^2$

Basis expansion

$$H|\psi_h\rangle = E_h|\psi_h\rangle$$

Here $H = T + V$ is the Hamiltonian operator. T is kinetic energy, V is potential energy.

- Choose a basis with a finite truncation $\{|\phi_1\rangle, |\phi_2\rangle, \cdots, |\phi_N\rangle\}$
- Expand the state vector in the basis,

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

The TISWE becomes a generalized matrix eigenvalue problem,

$$\sum_j H_{ij} c_j = E \sum_j w_{ij} c_j$$

where $H_{ij} \equiv \langle\phi_i|\hat{H}|\phi_j\rangle$, $w_{ij} \equiv \langle\phi_i|\phi_j\rangle$. In wave function representation,

$$\langle\phi_i|\hat{H}|\phi_j\rangle = \int \mathrm{d}^3x \int \mathrm{d}^3x' \phi_i(\vec{x}) H(x, x') \phi_j^*(\vec{x}')$$

- Solve the matrix eigenvalue equation using eigensolvers

Nystrøm method

$$\frac{p^2}{2m}\psi(p) + \int \frac{\mathrm{d}p'}{2\pi} V(p,p')\psi(p') = E\psi(p)$$

- Choose a set of Gaussian quadrature points $\{p_1, p_2, \cdots, p_N\}$
- Represent the integral using Gaussian quadratures ($\psi_i \equiv \psi(p_i)$),

$$\int \mathrm{d}p' V(p,p')\psi(p') \approx \sum_i w_i V(p,p_i)\psi_i$$

Then, the TISWE becomes,

$$\frac{p_i^2}{2m}\psi_i + \frac{1}{2\pi}\sum_j w_j V_{ij}\psi_j = E\psi_i$$

- Solve the eigenvalue problem $\sum_j H_{ij}v_j = Ev_i$, where, $v_i = \sqrt{w_i}\psi_i$, and $H_{ij} = \delta_{ij}(p_i^2/2m) + (1/2\pi)\sqrt{w_i w_j}V_{ij}$.

Example: Yukawa potential

$$\left[\frac{\vec{p}^2}{2m_r} - \alpha\frac{\exp(-\mu r)}{r}\right]\psi(\vec{r}) = E\psi(\vec{r}).$$

In momentum space,

$$\frac{\vec{p}^2}{2m_r}\psi(\vec{p}) - \int \frac{\mathrm{d}^3p'}{(2\pi)^3}\frac{4\pi\alpha}{(\vec{p}-\vec{p}')^2+\mu^2}\psi(\vec{p}') = E\psi(\vec{p}).$$

Separation of variables, $\psi(\vec{p}) = R(p)Y_{lm}(\hat{p})$

$$\frac{p^2}{2m_r}R(p) - \frac{4\alpha}{\pi}\int \mathrm{d}p' K_l(p,p')R(p') = ER(p).$$

where,

$$K_l(p,p') = \int_0^\infty \mathrm{d}r\, j_l(pr)re^{-\mu r}j_l(p'r)$$

For example ($\lambda = \mu/m_r$),

$$K_0(p,p') = \frac{1}{4pp'}\ln\left[\frac{(p+p')^2+\lambda^2}{(p-p')^2+\lambda^2}\right]$$

Numerical solution of non-relativistic Yukawa model

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October 11, 2016

Abstract

These notes describe a numerical method for solving Schrödinger equation with the Yukawa potential. Energy eigenvalues and wave functions are obtained and compared with the Coulomb results.

Introduction The Yukawa potential (aka. screened Coulomb potential) $V(r) = -(\alpha/r)\exp(-\mu r)$ is a universal potential for interactions mediated by massive particles in the non-relativistic limit. It is also useful for describing interactions in the medium – the "screened Coulomb interaction". Thus it is very important to find the solutions for the Yukawa potential in non-relativistic Schroedinger equation:

$$\Big[-\frac{\nabla^2}{2m} - \frac{\alpha}{r}e^{-\mu r}\Big]\psi(\vec{r}) = E\,\psi(\vec{r}), \tag{1}$$

where m is the reduced mass, $\alpha \equiv g^2/(4\pi)$ is the strength of the interaction with g the "charge", μ is the mass of the exchanged particle, and $\mu = 0$ gives the Coulomb potential. Alas, the above eigenvalue problem does not admit analytic solution, except for the Coulomb case.

In the momentum space, the eigenvalue equation becomes an integral equation:

$$\frac{\vec{p}^2}{2m}\psi(\vec{p}) - \int \frac{\mathrm{d}^3p'}{(2\pi)^3}\frac{4\pi\alpha}{(\vec{p}-\vec{p}')^2+\mu^2}\psi(\vec{p}') = E\,\psi(\vec{p}). \tag{2}$$

Here $\psi(\vec{p})$ represents the momentum-space wave functions, related to the coordinate-space wave function $\psi(\vec{r})$ by a Fourier transformation,

$$\psi(\vec{p}) = \int \mathrm{d}^3r\, e^{i\vec{p}\cdot\vec{r}}\psi(\vec{r}), \qquad \psi(\vec{r}) = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, e^{-i\vec{p}\,r}\psi(\vec{p}). \tag{3}$$

We have abused the notation ψ for wave functions. The wave functions are normalized according to

$$\int \mathrm{d}^3r\,\psi^*(\vec{r})\psi(\vec{r}) = 1, \qquad \int \frac{\mathrm{d}^3p}{(2\pi)^3}\psi^*(\vec{p})\psi(\vec{p}) = 1. \tag{4}$$

Before employing numerical methods, let us first put the equation to a dimensionless form. The natural scale in the problem is the Bohr radius ($\hbar = c = 1$): $a \equiv 1/(\alpha m)$. We also define: $\lambda \equiv a\mu$, $\kappa \equiv 2mEa^2 = 2E/(m\alpha^2) \equiv E/E_B$, with $E_B \equiv \alpha^2 m/2$ being the ground state binding energy within the Coulomb potential ($\mu = 0$). Upon substitutions: $\vec{p} \to a\vec{p}$, $\vec{r} \to \vec{r}/a$, $\psi(\vec{r}) \to a^{\frac{3}{2}}\psi(\vec{r}/a)$, $\psi(\vec{p}) \to a^{-\frac{3}{2}}\psi(a\vec{p})$, the Schrödinger equation and its momentum representation becomes,

$$\Big[-\nabla^2 - \frac{2}{r}e^{-\lambda r}\Big]\psi(\vec{r}) = \kappa\,\psi(\vec{r}), \tag{5}$$

$$\vec{p}^2\psi(\vec{p}) - \int \frac{\mathrm{d}^3p'}{(2\pi)^3}\frac{8\pi}{(\vec{p}-\vec{p}')^2+\lambda^2}\psi(\vec{p}') = \kappa\,\psi(\vec{p}). \tag{6}$$

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The theory has a rotational symmetry and the wave functions can be written as,

$$\psi(\vec{r}) = R(r)Y_{lm}(\hat{r}), \quad \psi(\vec{p}) = P(p)Y_{lm}(\hat{p}), \tag{7}$$

where Y_{lm} are the spherical harmonics. They are the eigenfunction of the angular momentum squared operator $\vec{L}^2$, and are normalized:

$$\int \mathrm{d}^2\Omega(\hat{r})Y^*_{l'm'}(\hat{r})Y_{lm}(\hat{r}) = \delta_{ll'}\delta_{mm'}. \tag{8}$$

As a result, we only need to solve for the radial part $R(r)$ or $P(p)$ which are real functions[1]. These radial wave functions are related by Hankel transformation:

$$R(r) = \frac{(-i)^\ell}{8\pi^3}\int_0^\infty \mathrm{d}p\, p^2 j_\ell(pr)P(p), \tag{9}$$

$$P(p) = i^\ell \int_0^\infty \mathrm{d}r\, r^2 j_\ell(pr)R(r). \tag{10}$$

Here $j_\ell(z)$ is the spherical Bessel function of the first kind, $\ell = 0, 1, 2, \cdots$ is the orbital angular momentum quantum number. The radial wave function are normalized according to:

$$\int_0^\infty \mathrm{d}r\, r^2 R^2(r) = 1, \tag{11}$$

$$\frac{1}{8\pi^3}\int_0^\infty \mathrm{d}p\, p^2 P^2(p) = 1. \tag{12}$$

Numerical Methods The coordinate-space Schroedinger equation can be written in the spherical coordinates:

$$\Big[-\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\frac{\mathrm{d}}{\mathrm{d}r}) + \frac{l(l+1)}{r^2} - \frac{2}{r}e^{-\lambda r}\Big]R(r) = \kappa\, R(r). \tag{13}$$

$$\Leftrightarrow \Big[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} - \frac{2}{r}e^{-\lambda r}\Big]u(r) = \kappa\, u(r), \tag{14}$$

where $u(r) = rR(r)$. The above differential equations can be discretized and solved numerically. In particular, in the case of an even-spacing grid[2],

$$\frac{\mathrm{d}}{\mathrm{d}r}f(r) = \frac{f(r+h) - f(r-h)}{2h} + \mathrm{O}(h^2) \tag{15}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}f(r) = \frac{f(r+h) - 2f(r) + f(r-h)}{h^2} + \mathrm{O}(h^2). \tag{16}$$

The obtained matrix can be diagonalized.

In these notes, however, we will focus on the momentum space representation and its numerical solutions. In momentum space, Schroedinger equation can be written as

$$p^2P(p) - \frac{4}{\pi}\int_0^\infty \mathrm{d}p'\, p'^2 K_\ell(p,p')P(p') = \kappa\, P(p), \tag{17}$$

where

$$K_\ell(p,p') \equiv \int_0^\infty \mathrm{d}r\, r\exp(-\lambda r)j_\ell(pr)j_\ell(p'r). \tag{18}$$

[1] $R(r)$ and $P(p)$ depends on the orbital quantum number l. The dependence is suppressed here.

[2] For non-even-spacing grids useful for radial wave functions, either a cutoff or a mapping is necessary before the discretization.

The above integral (18) can be evaluated analytically. The expressions for the first few K_ℓ are:

$$K_0(p,p') = \frac{1}{4pp'} \log\Big[\frac{(p+p')^2+\lambda^2}{(p-p')^2+\lambda^2}\Big]; \tag{19}$$

$$K_1(p,p') = \frac{p^2+p'^2+\lambda^2}{4p^2p'^2} \log\Big[\frac{(p+p')^2+\lambda^2}{(p-p')^2+\lambda^2}\Big] - \frac{1}{2pp'}; \tag{20}$$

$$K_2(p,p') = \frac{3p^4+2p^2p'^2+3p'^4+6(p^2+p'^2)\lambda^2+3\lambda^4}{16p^3p'^3} \log\Big[\frac{(p+p')^2+\lambda^2}{(p-p')^2+\lambda^2}\Big] - \frac{3(p^2+p'^2+\lambda^2)}{8p^2p'^2}. \tag{21}$$

Eq. (18) can also be evaluated numerically using quadrature method as described below.

Once K_ℓ is obtained, the integral in Eq. (17) can be approximated using quadrature method. For a general integral,

$$\int \mathrm{d}x\, f(x) = \sum_{i=1}^{N} w_i f(x_i) + R[f^{(2N+1)}(\xi)] \tag{22}$$

where x_i and w_i are pre-chosen abscissas and weights. For the radial integrals (17–18), the abscissas and weights can be obtained from the Gauss-Legendre quadrature with a mapping function. Gauss-Legendre quadrature approximates integrals over the interval $(-1,+1)$:

$$\begin{aligned} &\int_{-1}^{+1} \mathrm{d}z\, f(z) = \sum_{i=1}^{N} \omega_i\, f(x_i) + R[f^{(2N+1)}(\xi)]. \\ \Leftrightarrow &\int_{0}^{1} \mathrm{d}z\, f(z) = \sum_{i=1}^{N} \frac{1}{2}\omega_i\, f((x_i+1)/2) + R[f^{(2N+1)}(\xi)]. \end{aligned} \tag{23}$$

Here x_i are the zeros of Legendre polynomial $P_N(z)$, and $\omega_i \equiv 2(1-x_i^2)/(N+1)^2/[P_{N+1}(x_i)]^2$. We employ a mapping function $\phi : (0,1) \to (0,\infty)$:

$$r_i = \phi(\tfrac{1}{2}(x_i+1)), \quad w_i = \tfrac{1}{2}\omega_i\, \phi'(\tfrac{1}{2}(x_i+1)). \tag{24}$$

Now,

$$\int_0^\infty \mathrm{d}z\, f(z) = \sum_{i=1}^{N} w_i f(r_i) + R[f^{(2N+1)}(\xi)]. \tag{25}$$

We choose $r = x/(1-x)$. Other popular choices include: $r = a\tan(x\pi/2)$, $r = a(1-e^{-bx})/(e-e^x)$. While in principle the converged result is independent of the mapping function ϕ, the choice of it is very important in practice, as it controls the rate of convergence. It should be chosen to cover the extent of the wave function. Because different states have different radial extent, it is often difficult to come up with a universal mapping function optimal for all excited states. Fortunately, in most practical cases, we are interested in the first lowest states, whose radial extent is not far from the ground state.

The integral equation (17) can be written as,

$$p_i^2 P(p_i) - \frac{4}{\pi} \sum_j w_j p_j^2 K_\ell(p_i,p_j) P(p_j) = \kappa\, P(p_i). \tag{26}$$

It is convenient to define $v_i \equiv \sqrt{w_i} p_i P(p_i)$, with normalization[3]

$$\sum_i v_i^2 = 1. \tag{27}$$

Then, the discretized equation becomes,

$$\sum_j H_{ij} v_j = \kappa\, v_i, \quad H_{ij} = \delta_{ij} p_i^2 - (4/\pi)\sqrt{w_i w_j}\, p_i p_j\, K_\ell(p_i,p_j). \tag{28}$$

H is obviously Hermitian. The energy eigenvalue and the wave functions can be obtained by numerically diagonalizing the Hamiltonian matrix (see Fig. 1). The system can be solved in different quadrature order N. The continuum limit can be reach by extrapolating the quadrature order $N \to \infty$.

[3] We dropped a factor $1/\sqrt{8\pi^3}$ here.

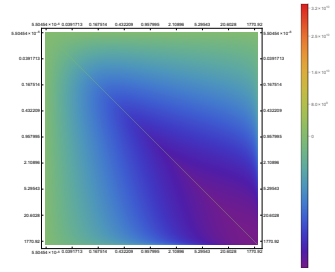


Figure 1: Visualization of the Hamiltonian matrix (28), with $\ell = 0$ (S-wave) and quadrature order $N = 512$.

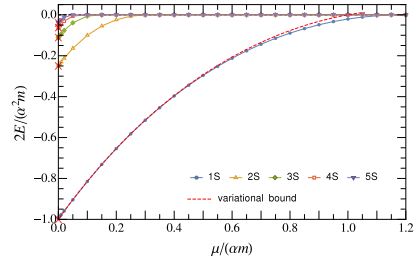


Figure 2: The S-wave energy eigenvalues as a function of μ. The values are obtained by extrapolating results over quadrature grids of the order $N = 16, 32, 64, 128, 512, 1024$. The red crosses represent Coulomb energy levels $E_n^{(\mathrm{coul})} = -\alpha^2 m/(2n^2)$, $n = 1, 2, 3, \cdots$. The red dashed line represents the upper bound obtained from variational method, using the Coulomb wave function as trial functions.

Results The obtained energy eigenvalues as a function of the exchanged particle mass μ are shown in Fig. 2 (see also Table 1). At small μ, the binding energies approach to the standard Coulomb values $E_n^{(\mathrm{coul})} = -\alpha^2 m/(2n^2)$ where $n = 1, 2, 3, 4, \cdots$ is the principle quantum number. The ground state energy is also in good agreement with the upper bound obtained from the variational method, using the Coulomb wave function as trial functions. As μ increases, bound states gradually disappear. The ground state starts to dissociate at $\mu \gtrsim \alpha m$.

The momentum-space wave functions can be extracted from the obtained eigenvectors. Fig. 3 presents an exertion of the S-wave wave functions. At small μ, the wave functions agree with the analytic results of the Coulomb potential:

$$\psi_{nl}^{(\mathrm{coul})}(p) = \mathcal{N}_{nl} \frac{p^l}{(1+n^2p^2)^{l+2}} C_{n-l-1}^{l+1}\left(\frac{n^2p^2-1}{n^2p^2+1}\right), \qquad (n = 1, 2, 3, \cdots; l = 0, 1, 2, 3, \cdots) \tag{29}$$

where $C_n^{\alpha}(z)$ is the Genebauer polynomial. As μ increases, the wave function within the momentum space becomes narrower. Furthermore, the change in excited wave functions are more dramatic comparing to that of the ground state as μ increases.

Summary We have described and demonstrated, in these notes, a numerical method to solve the non-relativistic Yukawa model. Both the energy eigenvalues and the wave functions agree with the Coulomb

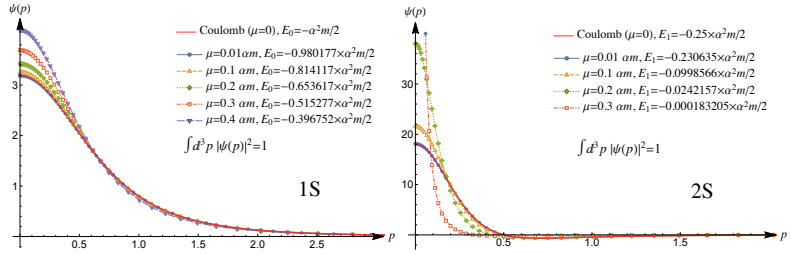


Figure 3: The obtained 1S and 2S wave functions in momentum space for selected μ. The red solid curves are the corresponding Coulomb results ($\mu = 0$).

Table 1: The energy eigenvalues E (in unit of $\alpha^2 m/2$) for different μ (in unit of αm).

$\mu/(\alpha m)$	$E_1/(\alpha^2 m/2)$	$E_2/(\alpha^2 m/2)$	$E_3/(\alpha^2 m/2)$	$E_4/(\alpha^2 m/2)$	$E_5/(\alpha^2 m/2)$
0	-1	-0.25	-0.1111	-0.0625	-0.04
0.0001	-0.9947	-0.2494	-0.1129	-0.06564	-0.04005
0.0005	-0.9907	-0.2466	-0.1096	-0.06165	-0.03953
0.001	-0.9892	-0.2454	-0.1084	-0.06114	-0.03823
0.002	-0.9877	-0.2438	-0.1065	-0.05891	-0.03742
0.005	-0.9837	-0.2389	-0.1014	-0.05365	-0.03145
0.01	-0.9762	-0.2302	-0.09269	-0.04533	-0.02440
0.02	-0.9591	-0.2125	-0.07643	-0.03123	-0.01249
0.05	-0.9043	-0.1638	-0.03889	-0.006285	-0.00002863
0.10	-0.8149	-0.1000	-0.006451		
0.15	-0.7315	-0.05453			
0.20	-0.6540	-0.02425			
0.25	-0.5821	-0.006805			
0.30	-0.5154	-0.0001847			
0.35	-0.4538				
0.40	-0.3968				
0.45	-0.3444				
0.50	-0.2963				
0.55	-0.2523				
0.60	-0.2123				
0.65	-0.1761				
0.70	-0.1437				
0.75	-0.1148				
0.80	-0.08942				
0.85	-0.06739				
0.90	-0.04863				
0.95	-0.03306				
1.00	-0.02057				
1.05	-0.01111				
1.10	-0.004575				
1.15	-0.0009122				
1.20					

results as small μ. These results can be used to compare with the Yukawa model in quantum field theories in the non-relativistic limit. The numerical method employed here can be adapted to solving integral equations appearing in the quantum field theoretical treatment of the Yukawa model.

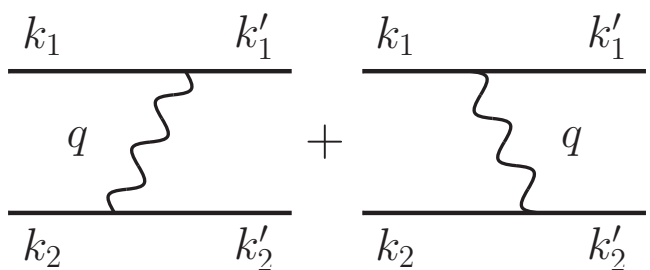
One-gluon-exchange on the light front

$$\left[\frac{\vec{k}_\perp^2+m_q^2}{x}+\frac{\vec{k}_\perp^2+m_{\bar{q}}^2}{1-x}+V\right]\psi(x,\vec{k}_\perp)=M_h^2\psi(x,\vec{k}_\perp)$$

The one-gluon-exchange interaction,

$$V_{\mathrm{OGE}}\circ\psi(x,\vec{k}_\perp)=\int\frac{\mathrm{d}x'}{2x'(1-x')}\int\frac{\mathrm{d}^2k'_\perp}{(2\pi)^3}\frac{4\pi\alpha(Q^2)}{Q^2}\psi(x',\vec{k}_\perp)$$

where $Q^2=\frac{1}{2}\left(\sqrt{\frac{x'}{x}}\vec{k}_\perp-\sqrt{\frac{x}{x'}}\vec{k}'_\perp\right)^2+\frac{1}{2}\left(\sqrt{\frac{1-x'}{1-x}}\vec{k}_\perp-\sqrt{\frac{1-x}{1-x'}}\vec{k}'_\perp\right)^2+\frac{1}{2}m^2(x-x')^2\left(\frac{1}{xx'}+\frac{1}{(1-x)(1-x')}\right)+\mu^2$.



Further readings

1. Yang Li, ``Numerical solution of non-relativistic Yukawa model'', private notes (2016).
2. M. van Iersel, C. F. M. van der Burgh and B. L. G. Bakker, ``Techniques for solving bound state problems,'' [arXiv:hep-ph/0010243 [hep-ph]].
3. M. Van Iersel, B. L. G. Bakker and F. Pijlman, ``Relativistic bound state calculations in light front dynamics,'' Nucl. Phys. B Proc. Suppl. **108**, 270-272 (2002) doi:10.1016/S0920-5632(02)01343-9 [arXiv:hep-ph/0202148 [hep-ph]].
4. G. 't Hooft, ``A Two-Dimensional Model for Mesons,'' Nucl. Phys. B **75**, 461-470 (1974)
5. Y. z. Mo and R. J. Perry, ``Basis function calculations for the massive Schwinger model in the light front Tamm-Dancoff approximation,'' J. Comput. Phys. **108**, 159-174 (1993).
6. S. S. Chabysheva and J. R. Hiller, ``Dynamical model for longitudinal wave functions in light-front holographic QCD,'' Annals Phys. **337**, 143-152 (2013); [arXiv:1207.7128 [hep-ph]].

Exercise II

Problem II-1: Solve problems I-1.1,I-1.2, I-2.1 using the methods you learned

Problem II-2: A quark model for meson. In the leading order, the inter-quark potential can be described by the superposition of a linear confining interaction $V_{\text{con}} = \sigma r$ and the Coulomb part $V_{\text{Coul}} = -(C_F \alpha_s / r)$, where $C_F = (4/3)$ is the color factor. In practical applications, the confining potential is ``screened'' at large distance to take into account the effect of string breaking at large excitations. The screened potential is, $V_{\text{scr}} = \sigma \mu^{-1} \left[1 - \exp(-\mu r)\right]$.

The non-relativistic Schrödinger equation of the above described quark model is,

$$\left[\frac{\vec{p}^2}{2m_r} + \frac{\sigma}{\mu}(1 - e^{-\mu r}) - \frac{4}{3}\frac{\alpha_s}{r}\right]\psi(\vec{r}) = E\psi(\vec{r}).$$

Solve this equation for eigenvalues and wave functions. Apply this model to charmonia. Find the best parameters and compare the results with the experiments.

Problem II-3: Solve problem I-2.2 using the methods you learned

Discussion on August 27, 2021

Tools

Hardwares

- Personal computer (PC, Mac, tablet): portability, accessibility
- Tower, personal workstation: accessibility, initial computational power
- Local cluster, server, cloud service, grid: accessibility, computational power
- Supercomputer, cloud: ultimate computational power with scalability

Softwares

- Integrated computational systems: Mathematica/Wolfram Alpha, Matlab, SciPy/NumPy, R, Octave, Julia, Sage
- Batch tools: bash, python, Mathematica, Matlab, GO, ROOT, ...
- Low level programming languages: C/C++, Fortran
- Data visualization: Mathematica, Origin, matlab, python, ...
- Editors: Vim, emacs, TeXlive, Word, notepad, sublime, Markdown, ...

Nystrøm method - revisited

Nystrøm method to solve Schrödinger wave equation:

$$\frac{p^2}{2m}\psi(p) + \int \frac{\mathrm{d}p'}{2\pi} V(p,p')\psi(p') = E\psi(p)$$

$$\Rightarrow \quad \frac{p_i^2}{2m}\psi_i + \frac{1}{2\pi}\sum_j w_j V_{ij}\psi_j = E\psi_i$$

where $\{p_1, p_2, \cdots, p_n\}$ are quadrature abscissas. $\psi_i = \psi(x_i)$, $V_{ij} = V(p_i, p_j)$.

- The key ingredient of Nystrøm method is to use Gaussian quadrature to approximate numerical integrations.

$$\int_a^b \mathrm{d}x f(x) = \sum_{i=1}^n w_i f(x_i) + \frac{(b-a)^{2n+1}(n!)^4 f^{(2n)}(\xi)}{(2n+1)[(2n)!]^3}, \ (a < \xi < b)$$

  The quadrature abscissas x_i are zeros of some orthogonal polynomials, w_i are weights. Example: Gauss-Legendre quadrature, $w_i = 2/(1-x_i^2)[P_n'(x_i)]^2$.

- Gaussian quadrature is exact for polynomials of degree less than $2n-1$.

Nystrøm method seeks a polynomial approximation of the wave functions.

Nystrøm method - revisited

Nystrøm method seeks to a polynomial approximation of the wave functions,

$$\psi(x) \to \hat{\psi}(x) = \sum_i \psi_i \ell_i(x), \quad (\hat{\psi}(x_i) = \psi_i)$$

- By definition, $\hat{\psi}(x_i) = \psi_i \Rightarrow \ell_i(x_j) = \delta_{ij}$
- $\ell_i(x)$ can be constructed from Lagrange interpolation polynomials, viz

$$\ell_i(x) = \prod_{j=1, i\neq j}^{n} \frac{x - x_j}{x_i - x_j}, \quad (\mathrm{deg}\ell_i(x) = n-1)$$

- Basis expansion: $\{|\phi_i\rangle\}$, with $\langle x|\phi_i\rangle = \mathcal{N}_i \ell_i(x)$.
- Inner product:

$$\langle \phi_i|\psi\rangle = \int \mathrm{d}x \phi_i^*(x)\hat{\psi}(x) = \sum_j w_j \mathcal{N}_i \overbrace{\ell_i(x_j)}^{\delta_{ij}} \psi(x_j) = \mathcal{N}_i w_i \psi(x_i)$$

- Schrödinger equation in this basis is the same as the Nystrøm equation.
- Evaluation of matrix elements becomes simple, even trivial.

Nystrøm method = basis method with Lagrange polynomial basis defined on quadrature mesh, aka. Lagrange mesh method (LMM) aka. discretized variable representation (DVR)

[D. Baye, Phys. Rep. 565, 1 (2015)]

General discussions, Q&A

Exercise III

For the problems as follow, consider the Gauss-Legendre quadrature as a concrete example. Properties of the Legendre polynomials can be found on Abramowitz & Stegun.

Problem III-1: Prove that

$$\ell_i(x) = \frac{P_n(x)}{a_{ni}(x - x_i)}$$

where $P_n(x)$ is the orthogonal polynomial. Find a_{ni}.

Problem III-2: Show that ℓ_i can be expanded using orthogonal polynomials P_k where $0 \leq k \leq n - 1$, viz

$$\ell_i(x) = \sum_{k=1}^{n-1} c_{ik} P_k(x).$$

Find c_{ik}.

References

1. Abramowitz, Milton; Stegun, Irene Ann, eds. (1983) [June 1964]. Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. Applied Mathematics Series. 55 (Ninth reprint with additional corrections of tenth original printing with corrections (December 1972); first ed.). Washington D.C.; New York: United States Department of Commerce, National Bureau of Standards; Dover Publications. ISBN 978-0-486-61272-0.
2. NIST Digital Library of Mathematical Functions
3. D. Baye, "The Lagrange-mesh method", Phys. Rep. 565, 1 (2015)

Discussion on Sept 10, 2021

General discussions

1. Pick at least one problem, and make a presentation to talk about how to solve it numerically

   15∼20 min, you can prepare some slides and/or notes to aid your presentation

   Let me know your preferred schedule

   While a right solution is our goal, we can also learn from mistakes

   Move fast and break things.

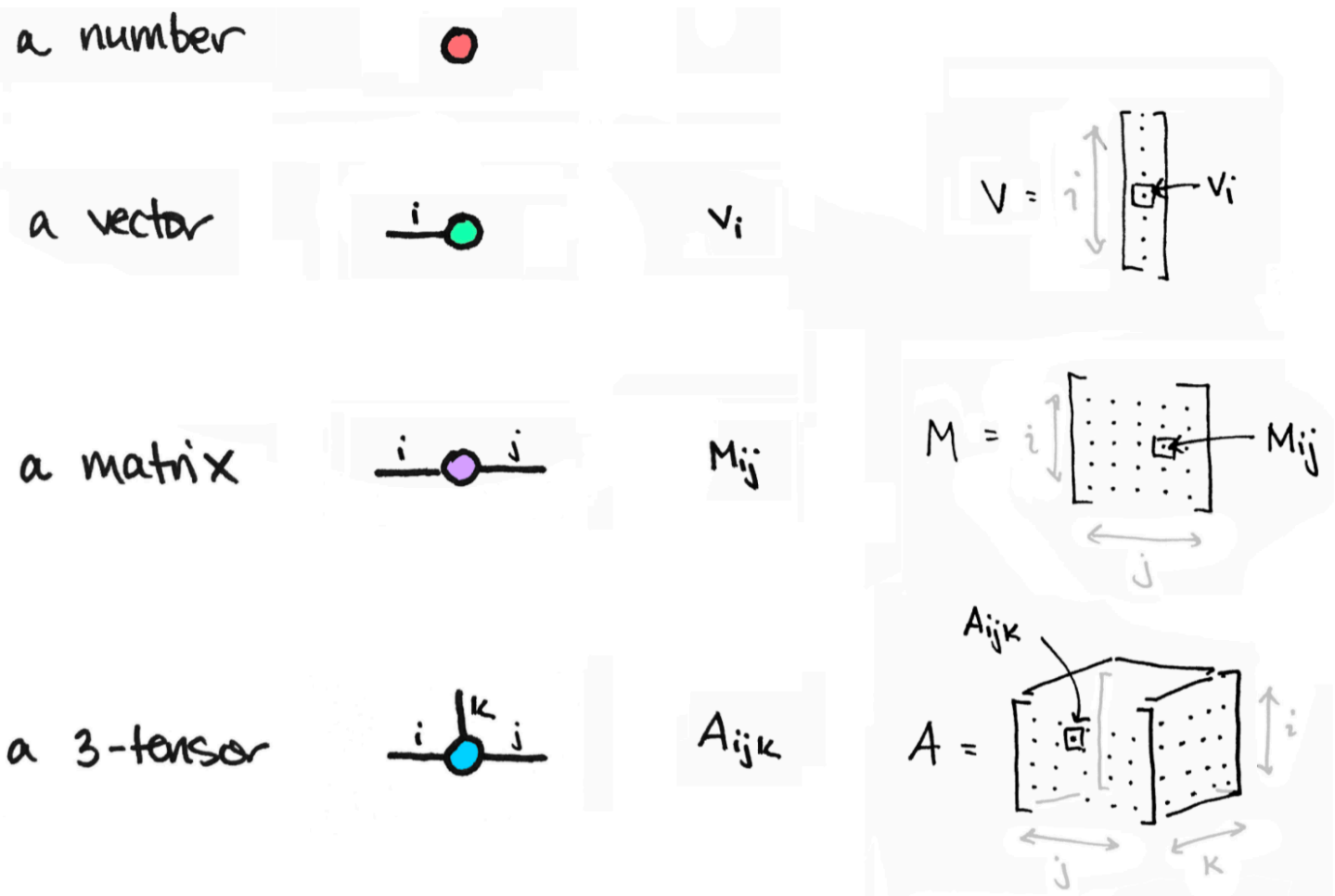
   Learning from breaking things.

2. Volunteer for today

3. Q&A

Matrix as diagrams

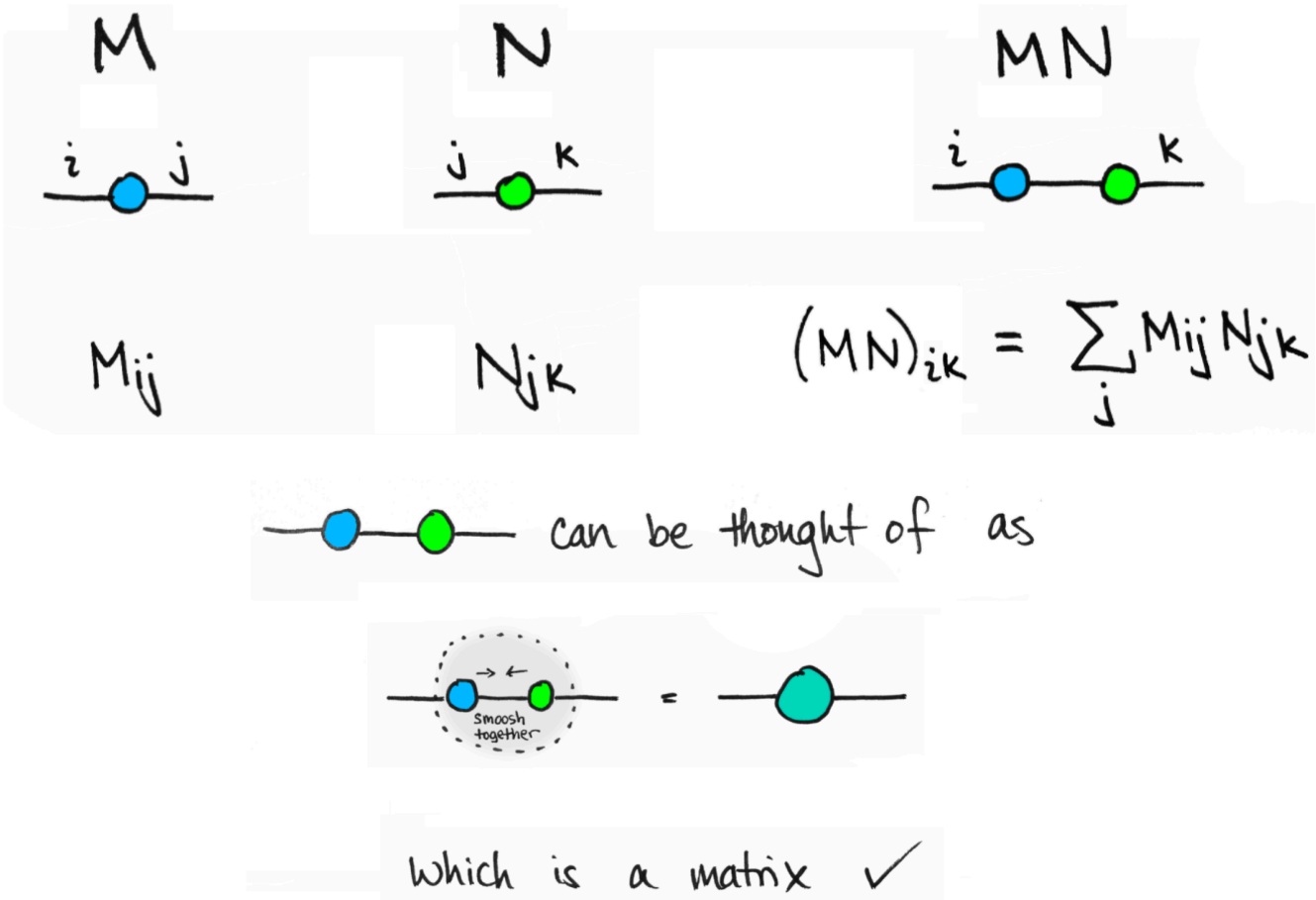
https://www.math3ma.com/blog/matrices-as-tensor-network-diagrams



Tensor network diagrams

Matrix as diagrams

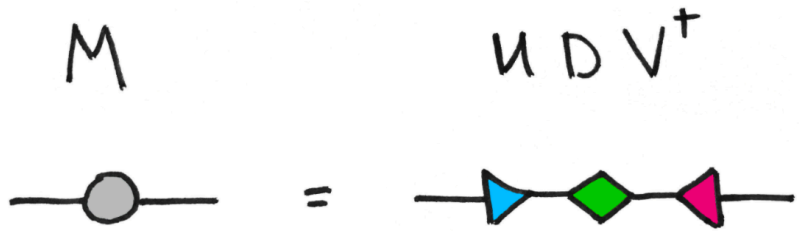
https://www.math3ma.com/blog/matrices-as-tensor-network-diagrams



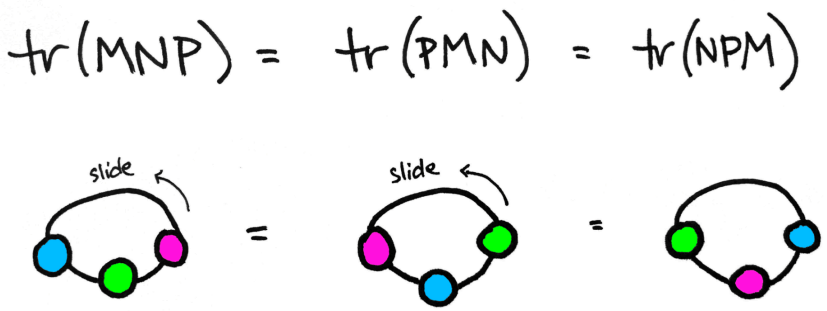
Matrix as diagrams

https://www.math3ma.com/blog/matrices-as-tensor-network-diagrams

SVD:



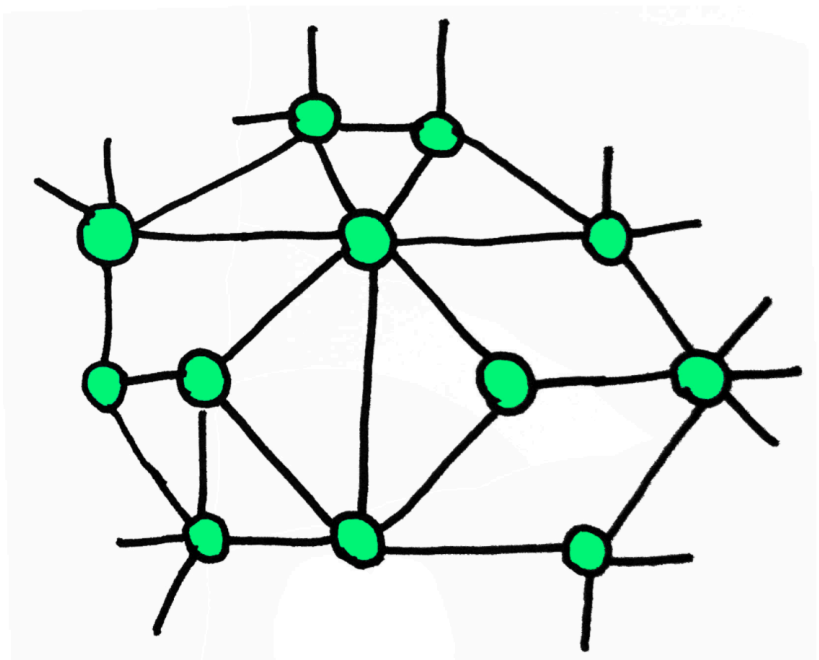
Trace identity:



Matrix as diagrams

`https://www.math3ma.com/blog/matrices-as-tensor-network-diagrams`

An awefully complicated tensor (network):



Diagrammatics for Schrödinger equation

$$H|\psi_n\rangle = E_n|\psi_n\rangle \tag{5}$$

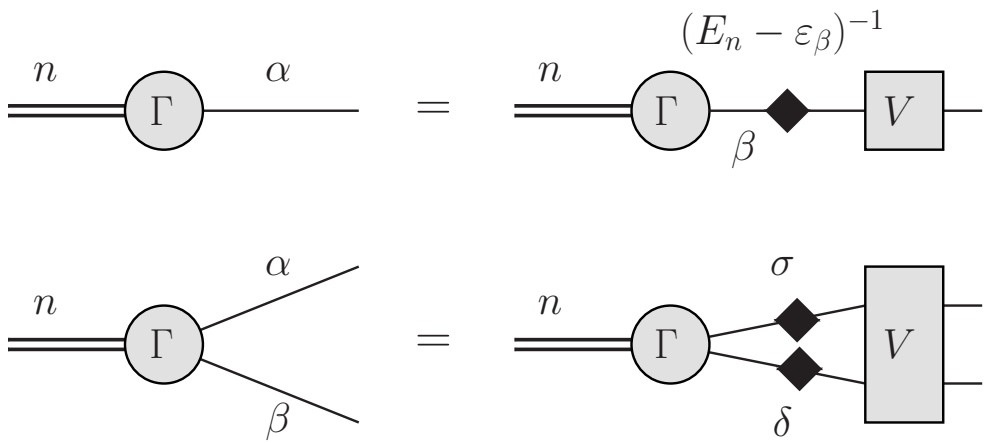
$$\Rightarrow \quad (H_0 + V)|\psi_n\rangle = E_n|\psi_n\rangle \qquad (H_0 \text{ is an ``simple'' Hamiltonian})$$

$$\Rightarrow \quad V|\psi_n\rangle = (E_n - H_0)|\psi_n\rangle$$

$$\Rightarrow \quad V(E_n + i\epsilon - H_0)^{-1}|\Gamma_n\rangle = |\Gamma_n\rangle \qquad |\Gamma_n\rangle \equiv (E_n - H_0)|\psi_n\rangle$$

$$\Rightarrow \quad \sum_\beta \frac{\langle\alpha|V|\beta\rangle\langle\beta|\Gamma_n\rangle}{E_n + i\epsilon - \varepsilon_\beta} = \langle\alpha|\Gamma_n\rangle \qquad \langle\alpha|H_0|\beta\rangle = \varepsilon_\alpha\delta_{\alpha\beta}$$

$$\Rightarrow \quad \sum_\beta \frac{V_{\alpha\beta}\Gamma_{\beta n}}{E_n + i\epsilon - \varepsilon_\beta} = \Gamma_{\alpha n} \qquad V_{\alpha\beta} \equiv \langle\alpha|V|\beta\rangle, \Gamma_{\alpha n} \equiv \langle\alpha|\Gamma_n\rangle$$



$$\Gamma^{(n+1)} = VG_0\Gamma^{(n)} \; (G_0 = (E - H_0)^{-1})$$

Examples:

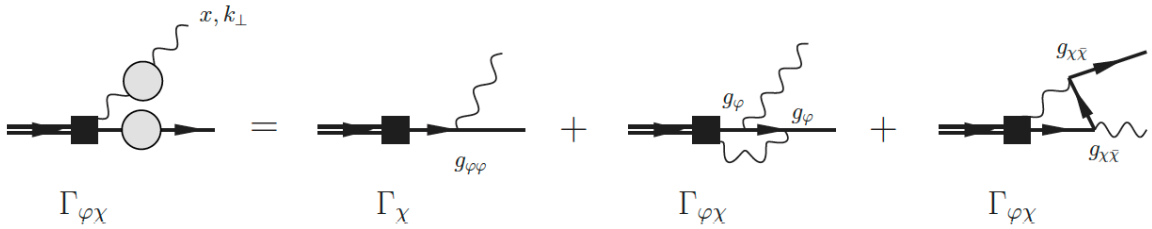
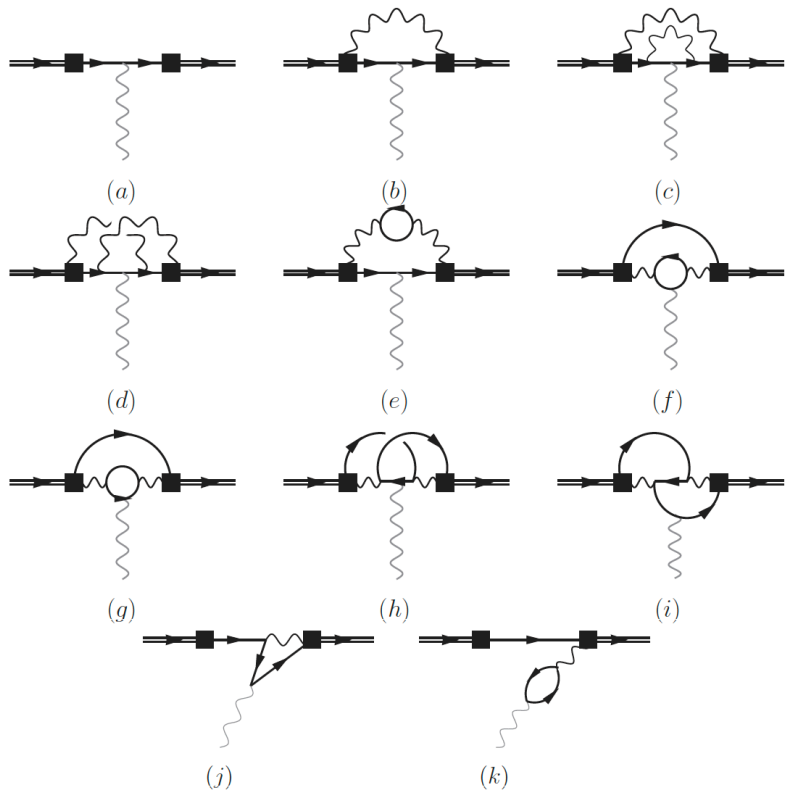


FIG. 12. The diagrammatic representation of Eq. (39).

$$\langle \Psi | J^\mu | \Psi \rangle$$



Discussion on Sept. 14, 2021

General discussions

- Schedule, plans
- `https://www.tensors.net`
- References on computational physics:
  - Thijssen, Computational Physics
  - Koonin, Computational Physics
  - Landau, A survy of computational physics
  - **丁泽军：计算物理讲义**
  - **马文淦：《计算物理学》**

  None of these will cover everything -- because there is no such thing as computational physics! Learn as needed
- Presentation: Duan

Matrix diagonalization

Diagonalization/eigenvalue equation is one of the most important methods in computational sciences

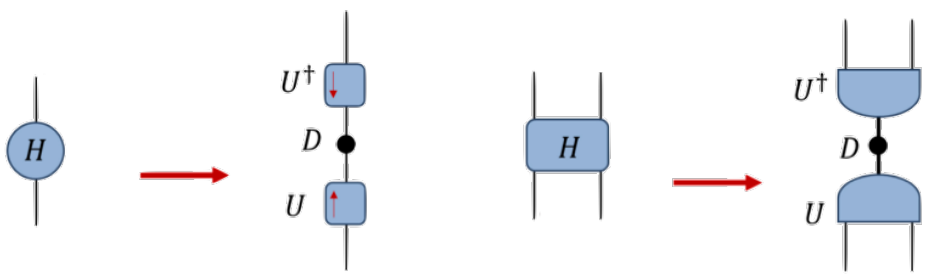
$$A \cdot v = \lambda v \tag{6}$$

For simplicity, we only consider Hermitian matrices.

- $A = U^\dagger \Lambda U$, such that $U^\dagger U = 1$, $\Lambda = \mathbf{diag}\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ is diagonal matrix, λ_i are A's eigenvalues.

$$U = [v_1, v_2, \cdots, v_n]$$

- Eigen decomposition: $A = \sum_i \lambda_i v_i v_i^\dagger$ or in Dirac's notation: $\underline{A} = \sum_i \lambda_i |v_i\rangle\langle v_i|$
- Eigenvectors form an orthonormal complete basis: $x = \sum_i c_i v_i, \forall$ vector x
- $\mathbf{det}(\lambda - A) = 0$



Power iteration

- Without too much loss of generality, $\lambda_1 > \lambda_2 > \lambda_3 > \cdots > 0$. The corresponding (orthonormalized) eigenvectors are, $v_1, v_2, \cdots$,
- Observe:

$$A^k \cdot x = \sum_i \lambda_i^n c_i v_i = \lambda_1^k \left[c_1 v_1 + \sum_{i=2} \left(\frac{\lambda_i}{\lambda_1} \right)^k c_i v_i \right] \xrightarrow{k \gg 1} \lambda_1^k c_1 v_1, \quad (7)$$

  - Assumption: maximum eigenvalue is non-generate
  - Convergence rate is controlled by $|\lambda_2 / \lambda_1|$
- Implementation:
  - Choose a normalized initial vector $x^{(0)}$ $\mathcal{O}(N)$
  - Compute $y^{(k+1)} := A \cdot x^{(k)}$ $\mathcal{O}(N^2)$
  - Compute $\lambda^{(k)} := y^{(k+1)} \cdot x^{(k)} = x^{(k)} \cdot A \cdot x^{(k)} \xrightarrow{k \gg 1} \lambda_1$ $\mathcal{O}(N)$
  - Normalize $y^{(k+1)}$: $x^{(k+1)} := \frac{y^{(k+1)}}{\|y^{(k+1)}\|} = \frac{A \cdot x^{(k)}}{\|A \cdot x^{(k)}\|} \xrightarrow{k \gg 1} v_1$ $\mathcal{O}(N)$
- Overall complexity: $\mathcal{O}(N^2 k)$

Power iteration: issues

Remaining issues of power iteration:

- How to get multiple and even all eigenpairs?
- Degenerate case $\lambda_1 = \lambda_2 = \cdots = \lambda_k$ $(k < n)$
- Smallest eigenvalue and eigenvectors

Power iteration: ground states

In Hamiltonian formalism, we wish to get the lowest lying eigenvalues and eigenstates.

- Lowest energy state is the ground states while the highest energy states are not useful (numerical noise)
- Method 1: shift
  - Consider $B = A - sI$ where s is close to the largest eigenvalue λ_1
  - Eigenvalues of B: $\lambda_1 - s, \lambda_2 - s, \cdots$
  - Magnitudes: $|\lambda_1 - s| < |\lambda_2 - s| < \cdots$ if s is close to λ_1
- Method 2: exponentiation
  - Consider $U = \exp(-A)$
  - Eigenvalues of U: $e^{-\lambda_1} < e^{-\lambda_2} < \cdots$
  - Power iteration $U^n = \exp(-nA)$

    Application: imaginary time evolution,

    $$|\psi(t)\rangle = \exp(-Ht)|\psi(0)\rangle \xrightarrow{t \gg \Delta E^{-1}} e^{-E_{gs}t}|\psi_{gs}\rangle$$

Successive power iterations

How to get multiple and even all eigenpairs: successive power iteration

- Redo the power iteration with a second vector x_2 and project out the obtained eigenvector v_1
  - Obtain v_1 from power iteration
  - Choose initial vector $x_2 := y_2 - (v_1^\dagger \cdot y_2)v_1 = \sum_{i=2} c_{i2} v_i$
  - Power iteration with x_2: $A^k \cdot x_2 = \sum_{i=2} \lambda_i^k c_{i2} v_i$
- Problem: if the orthogonalization is not complete due to numerical precision, $x_2 = \epsilon v_1 + \sum_{i=2} c_{i2} v_i$ ($|\epsilon| \ll |c_{i2}|$)

$$A^k \cdot x_2 = \epsilon \lambda_1^k v_1 + \sum_{i=2} \lambda_i^k c_{i2} v_i$$

  Only applicable if $|\epsilon| \ll |\lambda_2/\lambda_1|^k \ll 1$.
- Solution: re-orthogonalize the vector after n_{reo} iterations
  - $n_{\text{reo}} \ll \frac{\ln|\epsilon|}{\ln|\lambda_2/\lambda_1|}$
  - We can even take $n_{\text{reo}} = 1$ and re-orthogonalize every step

Simultaneous power iteration

Degenerate case $\lambda_1 = \lambda_2 > \lambda_3 > \cdots$

- Power iteration converges to a vector in the eigen-subspace instead of a single eigenvector

$$A^k \cdot x = \sum_i \lambda_i^n c_i v_i = \lambda_1^k \left[c_1 v_1 + c_2 v_2 + \sum_{i=3} \left(\frac{\lambda_i}{\lambda_1} \right)^k c_i v_i \right]$$
$$\xrightarrow{k \gg 1} \lambda_1^k (c_1 v_1 + c_2 v_2)$$

- We need two linearly independent initial vectors $x_1 = \sum_i c_{i1} v_i, x_2 = \sum_i c_{i2} v_i$

$$A^k \cdot x_1 \to \lambda^k (c_{11} v_1 + c_{21} v_2), \quad A^k \cdot x_2 \to \lambda^k (c_{12} v_1 + c_{22} v_2)$$

- Problem: linear independence may lose during iteration
  Example: construct x_1, x_2 *such that* $c_{12} = c_{22} = 0$, *but* $x_1 \cdot x_2 = 0$
- Solution: iterate x_1, x_2 simultaneously and re-orthgonalize every step

Orthogonal power iteration

Simultaneous power iteration with a re-orthogonalization can be generalized to n vectors which remarkably also include the successive iteration case

- In general, we can do simultaneous power iterative with an initial matrix $X = [x_1, x_2, \cdots, x_n]$

$$X = VC$$

where $V = [v_1, v_2, \cdots, v_n]$ is the eigen-vector matrix.

$$\begin{aligned} A^k \cdot X &= [\lambda_1^k v_1, \lambda_2^k v_2, \cdots, \lambda_n^k v_n]C \\ &= [\sum_j C_{j1}\lambda_j^k v_j, \sum_j C_{j2}\lambda_j^k v_j, \cdots, \sum_j C_{jn}\lambda_j^k v_j] \end{aligned}$$

- Re-orthogonalization $QR = X$ where $Q^\dagger Q = 1$, R is triangular.
- Implementation:
  - Choose a random initial matrix $X^{(0)}$
  - Re-orthonormalize $X^{(k)}$: $Q^{(k)}R^{(k)} = X^{(k)}$, $Q^{(k)}$ is orthogonal matrix, and $R^{(k)}$ is triangular.
  - Compute $X^{(k+1)} = AQ^{(k)}$. Then, $Q^{(k)} \to V$, $R^{(k)} \to \Lambda$

QR algorithm

- The celebrated QR algorithm is,
  - $A^{(0)} = A$
  - QR decomposition $A^{(k)}$: $Q^{(k)} R^{(k)} = A^{(k)}$, where $Q^{(k)}$ is orthogonal matrix, and $R^{(k)}$ is triangular.
  - Compute $A^{(k+1)} = R^{(k)} Q^{(k)} = [Q^{(k)}]^\dagger A^{(k)} Q^{(k)} \sim A^{(k)}$. Then, $Q^{(k)} \to V$, $A^{(k)} \to \Lambda$
- QR algorithm is equivalent to the orthogonal power iteration.
- The crucial step is the QR decomposition which effectively implements the re-orthogonalization.
- Computational complexity of QR decomposition is $\mathcal{O}(N^3)$ for general matrices and $\mathcal{O}(N)$ for tridiagonal matrices.
- QR decomposition can be implemented using (i) Householder transformations (ii) Givens rotations (iii) Gram-Schmidt procedure. N.B., Gram-Schmidt procedure is not numerically stable.

Numerical libraries: `LAPACK`

- Short for ``Linear Algebra Package'' is a standard numerical linear algebra library
- Functionalities: linear solver, linear least squares, eigenvalue problems, SVD, LU, QR, Shur decomposition, Cholesky decomposition
- Language: Fortran 77/90 (native), C binding, other language bindings are available through external libraries or wrappers
- Officially published by Netlib under BSD-new license (free): **`www.netlib.org/lapack/`**
- Also available in computational systems, e.g. intel's MKL, matlab, mathematica, ...
- Parallel versions: **`ScaLAPACK`**, **`PLAPACK`**

```
call dsyevx('V', 'I', 'U', dm, ham, dm, 0d0, 0d0, 1, nev,    &
            abstol, nnev, eval, evec, dm, work, lwork, iwork, &
            ifail, ierr)
```

Discussion on Sept. 24, 2021

Quantum theories

Schrödinger equation:

$$H|\psi_h\rangle = E_h|\psi_h\rangle$$

Some notable examples:

- Quantum few-body systems
- Quantum many-body systems
- Quantum fields
- Quantum gravity, string, brane and other unknown beasts

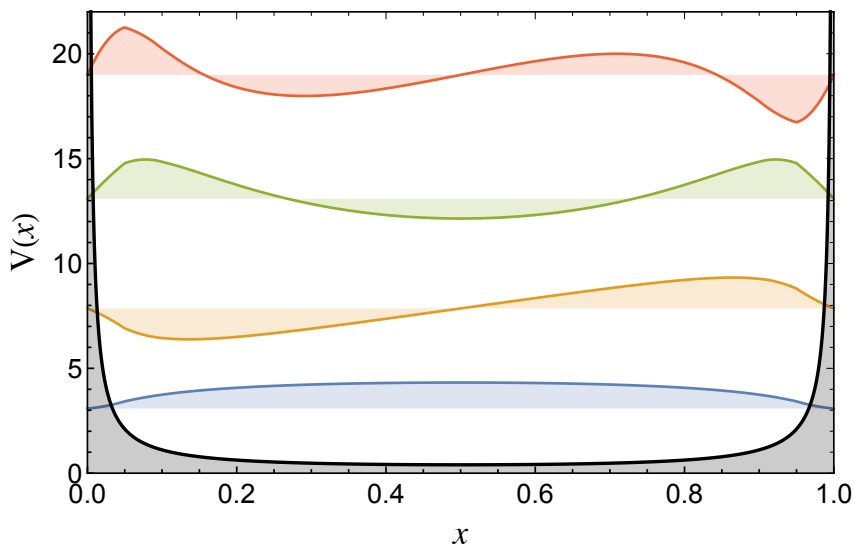
Schrödinger wave equation

Single-particle: $\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$

$$H = \frac{\vec{p}^2}{2m} + V(r)$$

Schrödinger wave equation:

$$\left[\frac{\vec{p}^2}{2m} + V(r) \right] \psi(\vec{r}) = E\psi(\vec{r})$$



Quantum many-body systems

Quantum many-body system:

$$H = \sum_i \frac{\vec{p}_i^2}{2m_i} + U(\vec{r}_i) + \frac{1}{2}\sum_{i,j} V(r_{ij}) + \frac{1}{3!}\sum_{i,j,k} V(r_{ijk}) + \cdots$$

- Coordinate or momentum space many-body wave function

$$\psi(\{\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_n\}) = \langle \{\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_n\} | \psi \rangle$$

- Self-bound systems: molecules, atoms, nuclei, hadrons, cold atoms
- Condensed matters: gas/plasma, lattice gas, fluids, soft matter, glass, solids
- Controlled systems: qbits, qgates, quantum simulator, quantum computer
- Second quantization and indistinguishable particles
  One-body operator:

$$O = \sum_{\alpha,\beta} O_{\alpha\beta} c_\alpha^\dagger c_\beta \qquad (O_{\alpha\beta} = \langle \alpha | O | \beta \rangle)$$

Quantum fields

Classical fields:

- Elasticity, electromagnetism, gravity
- Continuum limit of lattice models

$$q_i \to \varphi(\vec{x}), \quad p_i \to \pi(\vec{x})$$

- Lagrangian (density): $S = \int \mathrm{d}^4 x \, \mathscr{L}[\partial\varphi, \varphi]$
- Euler-Lagrangian equation
- Fluidity: local conservation laws $D_\mu T^{\mu\nu} = 0$
- Mode expansion:

$$\varphi(x) = \sum_\alpha \left[c_\alpha(t) u_\alpha(x) + c_\alpha^*(t) u_\alpha^*(x) \right]$$

Quantum fields

Quantum fields:

- Degrees of freedom: field operator φ (operator-valued distributions)
- Continuum limit is highly non-trivial due to quantum fluctuations

$$q_i \to \varphi(\vec{x}), \quad p_i \to \pi(\vec{x})$$

- Heisenberg representation, Euler-Lagrangian equation, Dyson-Schwinger equations and the covariant formulation
- Canonical quantization:

$$\left[p_i, q_j\right]_{t=0} = i\delta_{ij} \;\to\; \left[\pi(\vec{x}), \varphi(\vec{y})\right]_{t=0} = i\delta^3(x-y)$$

- Hamiltonian:

$$H = \int \mathrm{d}^3x \left\{ \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\nabla^2\varphi^2 + \tfrac{1}{2}m^2\varphi^2 - \tfrac{g}{4!}\varphi^4 \right\}$$

- Particles are eigenstates of the Hamiltonian (particle $\neq$ fields)

Quantum fields

Second quantization:

$$\varphi(x) = \sum_{\alpha} \left[c_\alpha u_\alpha(x) + c_\alpha^\dagger u_\alpha^*(x) \right]_{t=0}$$

- CCR: $\left[c_\alpha, c_\beta^\dagger\right] = \delta_{\alpha\beta}$
- Momentum rep'n:

$$\varphi(x) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2E_p} \left[a(p) e^{-ip\cdot x} + a^\dagger(p) e^{+ip\cdot x} \right]_{t=0}$$

  where $\left[c(p), c^\dagger(p')\right] = 2E_p (2\pi)^3 \delta^3(p - p')$
- Field Hamiltonian in second quantized form:

$$H = \sum_{\alpha\beta} \varepsilon_{\alpha\beta} c_\alpha^\dagger c_\beta - \frac{g}{4!} \sum_{\alpha\beta\delta\gamma} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

QFT ≈ QMBT

Discussion on Oct. 15, 2021

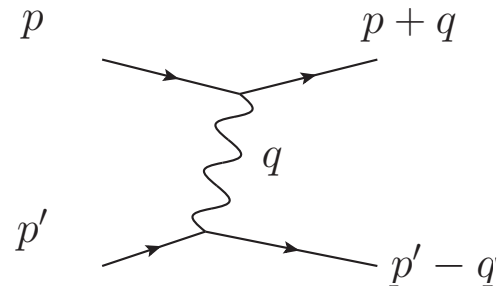
Quantum field theory and quantum many-body theory

QFT ≈ QMBT: QFT and QMBT can be related through second quantization.

Example: Many-body Hamiltonian:

$$H = \sum_i \frac{\vec{p}_i^2}{2m_i} + \sum_{i<j} V(r_{ij})$$

Second quantized many-body Hamiltonian:



$$\underline{H} = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \underline{a}_\sigma^\dagger(\vec{p}) \frac{\vec{p}^2}{2m} \underline{a}_\sigma(\vec{p}) + \sum_{\sigma,\sigma'} \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{\mathrm{d}^3 p'}{(2\pi)^3} \frac{\mathrm{d}^3 q}{(2\pi)^3} \underline{a}_\sigma^\dagger(\vec{p}+\vec{q}) \underline{a}_{\sigma'}^\dagger(\vec{p}'-\vec{q}) \widetilde{V}(q) \underline{a}_{\sigma'}(\vec{p}') \underline{a}_\sigma(\vec{p})$$

Rule of second quantization:

$$O_i^{[1]} = \sum_{\alpha,\beta} O_{\alpha\beta}^{[1]} c_\alpha^\dagger c_\beta \qquad (O_{\alpha\beta} = \langle\alpha|O_i^{[1]}|\beta\rangle),$$

$$O_{ij}^{[2]} = \sum_{\alpha,\beta,\rho\sigma} O_{\alpha\beta\rho\sigma}^{[2]} c_\alpha^\dagger c_\beta^\dagger c_\rho c_\sigma \qquad (O_{\alpha\beta\rho\sigma} = \langle\alpha\beta|O_{ij}^{[2]}|\rho\sigma\rangle)$$

Quantum field theory and quantum many-body theory

Hamiltonian quantum field theory:

$$\underline{H} = \int \mathrm{d}^3x \underline{\psi}^\dagger \frac{-\nabla^2}{2m} \underline{\psi} + \int \mathrm{d}^3x\, \mathrm{d}^3x' \underline{\psi}^\dagger(\vec{x}) \underline{\psi}^\dagger(\vec{x}') V(|\vec{x}-\vec{x}'|) \underline{\psi}(\vec{x}') \underline{\psi}(\vec{x})$$

Here, the field operator:

$$\underline{\psi}_\alpha(\vec{x}) = \sum_\sigma \int \frac{\mathrm{d}^3p}{(2\pi)^3} \chi_\alpha(\vec{p},\sigma) e^{i\vec{p}\cdot\vec{x}} \underline{a}_\sigma(\vec{p})$$

Here $\chi_\alpha(p,\sigma)$ is the ``spin wave function'' (spinor, polarization vector/tensor).

Classical Lagrangian (field theory):

$$\mathscr{L} = \frac{i}{2}(\partial_t \psi^\dagger \psi - \psi^\dagger \partial_t \psi) - \frac{1}{2m} \nabla\psi^\dagger \cdot \nabla\psi - \int \mathrm{d}^3x'\, \psi^\dagger(\vec{x}) \psi^\dagger(\vec{x}') V(|\vec{x}-\vec{x}'|) \psi(\vec{x}') \psi(\vec{x})$$

Canonical quantization: $\mathscr{L} \to H$

$- \int \mathrm{d}^3x'\, n(\vec{x}) n(\vec{x}') V(|\vec{x}-\vec{x}'|)$
+ normal ordered terms
$n(\vec{x}) \equiv \psi^\dagger(\vec{x})\psi(\vec{x})$

Quantum many-body theories

Important examples:

- Born-Oppenheimer electron gas:

$$H = \sum_i \frac{\vec{p}_i^2}{2m_i} + \frac{1}{2}\sum_{i,j}\frac{\alpha}{r_{ij}}$$

$$= \sum_{\vec{p},\lambda}\frac{p^2}{2m}a^\dagger_{\vec{p}\lambda}a_{\vec{p}\lambda} + \frac{1}{2V}\sum_{\vec{p},\lambda,\vec{p}',\lambda',\vec{q}}\frac{4\pi\alpha}{q^2}a^\dagger_{\vec{p}+\vec{q},\lambda}a^\dagger_{\vec{p}'-\vec{q},\lambda'}a_{\vec{p}',\lambda'}a_{\vec{p},\lambda}$$

- Bardeen–Cooper–Schrieffer liquids:

$$H = \sum_i\left(\frac{p_i^2}{2m_i} - \mu\right) + \frac{1}{2}\sum_{i,j}\frac{\alpha}{r_{ij}}$$

$$= \sum_{\vec{p},\lambda}\left(\frac{p^2}{2m} - \mu\right)a^\dagger_{\vec{p}\lambda}a_{\vec{p}\lambda} + \sum_{\vec{p},\vec{p}'}V(\vec{p},\vec{p}')a^\dagger_{\vec{p}\uparrow}a^\dagger_{-\vec{p}\downarrow}a_{-\vec{p}'\downarrow}a_{\vec{p}'\uparrow}$$

- Fermi-Hubbard model (Lattice gas):

$$H = -t\sum_\sigma\sum_{\langle i,j\rangle}\left(c^\dagger_{j\sigma}c_{i\sigma} + c^\dagger_{i\sigma}c_{j\sigma}\right) + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

Non-perturbative approaches

$$H = \sum_{\alpha,\beta} h_{\alpha\beta} c_\alpha^\dagger c_\beta + \sum_{\alpha,\beta,\rho,\sigma} v_{\alpha\beta,\rho\sigma} c_\alpha^\dagger c_\beta^\dagger c_\rho c_\sigma + \cdots$$

where $h_{\alpha\beta} \equiv \epsilon_\alpha \delta_{\alpha\beta} + u_{\alpha\beta}$.

- Perturbation theory $v \ll h$
- Non-perturbative approaches
  - Approximations:
    - Mean-field approach: Hatree-Fock (HF), Density function theory
    - Post HF: Tamm-Dancoff, Ramdom-phase approximation
  - Effective field theory
  - Direct methods:
    - Full Configuration Interaction
    - Coupled Cluster
    - Quantum Monte-Carlo
    - Hamiltonian similarity renormalization group
    - Density matrix renormalization group
  - New many-body techniques:
    - Quantum simulation and quantum computing
    - Tensor network representation
    - Deep learning

Assignments

Do a literature review on one of the following emerging techniques in quantum many-body theory and quantum field theory:

- Quantum simulation and quantum computing (Duan)
- Tensor network representation (Wang)
- Deep learning

Schedule a time for presentation.

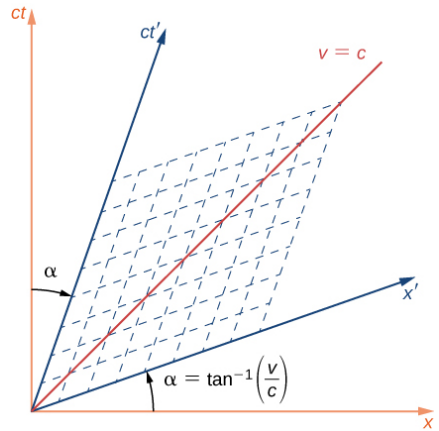
Difficulties with relativistic wave functions

- Wave function is frame dependence

  Rest-frame wave function ≠ moving frame wave function, boost transformation is dynamical (involves time-evolution)

  Lost of cluster decomposition, key property for renormalization

  Hadronic observables require wave functions at large $\vec{P}$: infinite momentum frame



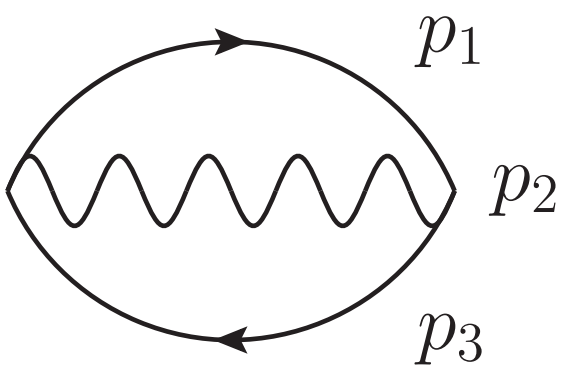
- Square root issues

  Square roots in kinetic energies and in energy denominators

$$H_{NR} = \sum_i \frac{\vec{p}_i^2}{2m_i} + \sum_{ij} V_{ij}$$

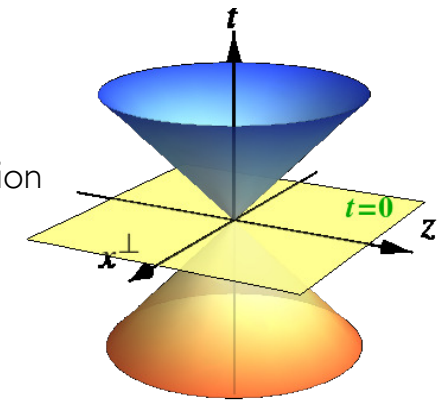
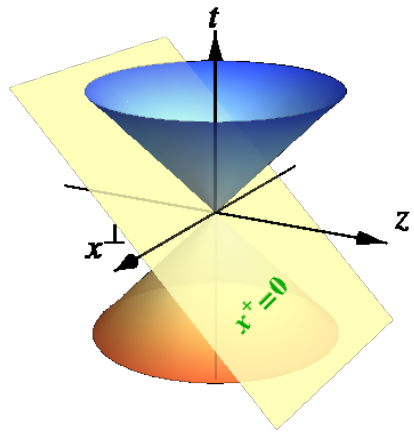
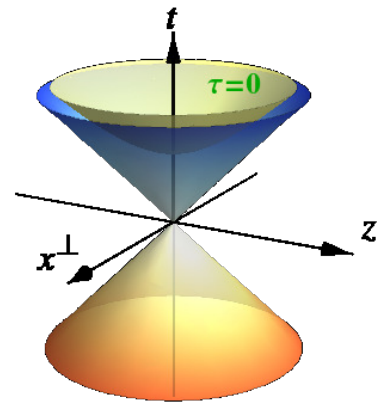
$$\rightarrow H_R = \sum_i \sqrt{\vec{p}_i^2 + m_i^2} + \sum_{ij} V_{ij}$$

- Vacuum pair production and annihilation



Dirac's forms of relativistic dynamics [Dirac, Rev. Mov. Phys. '49]

In Hamiltonian dynamics, time dictates the direction of the dynamical evolution. In relativity, $t = x^0$ is not the only choice of time.

	instant form	**front form**	**point form**
time variable	$t = x^0$	$x^+ \triangleq x^0 + x^3$	$\tau \triangleq \sqrt{t^2 - \vec{x}^2 - a^2}$
quantization surface			
Hamiltonian	$H = P^0$	$P^- \triangleq P^0 - P^3$	P^μ
kinematical	$\vec{P}, \vec{J}$	$\vec{P}^\perp, P^+, \vec{E}^\perp, E^+, J_z$	$\vec{J}, \vec{K}$
dynamical	$\vec{K}, P^0$	$\vec{F}^\perp, P^-$	$\vec{P}, P^0$
dispersion relation	$p^0 = \sqrt{\vec{p}^2 + m^2}$	$p^- = (\vec{p}_\perp^2 + m^2)/p^+$	$p^\mu = mv^\mu \ (v^2 = 1)$

$P^\pm \triangleq P^0 \pm P^3$, $\vec{P}^\perp \triangleq (P^1, P^2)$, $x^\pm \triangleq x^0 \pm x^3$, $\vec{x}^\perp \triangleq (x^1, x^2)$, $E^i = M^{+i}$, $E^+ = M^{+-}$, $F^i = M^{-i}$, $K^i = M^{0i}$, $J^i = \frac{1}{2}\epsilon^{ijk}M^{jk}$.

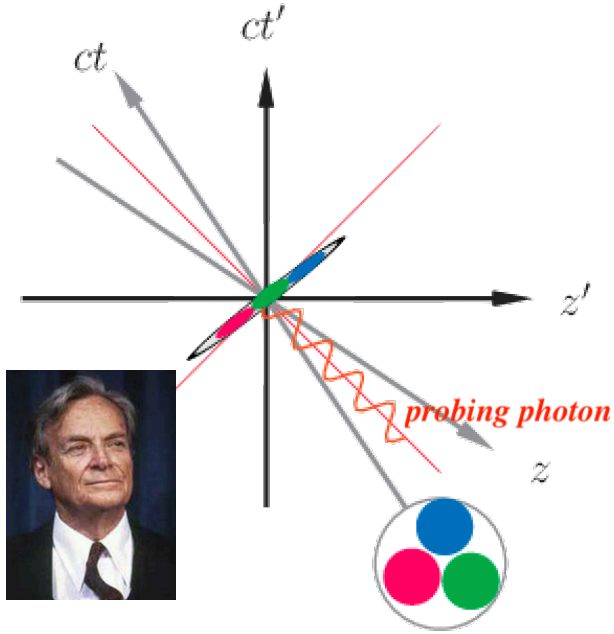
Advantages of light-front dynamics

	non-relativistic	relativistic	
		instant form	front form
kinetic energy	$\sum_i \frac{\vec{p}_i^2}{2m_i}$	$\sum_i \sqrt{\vec{p}_i^2 + m_i^2}$	$\sum_i \frac{\vec{p}_{i\perp}^2 + m_i^2}{p_i^+}$
Lorentz covariance	partial (rotation)	no	partial (boost)
frame dependence	no	yes	no
vacuum fluctuation	no	yes	no

Understanding physics on the light front

Infinite momentum frame

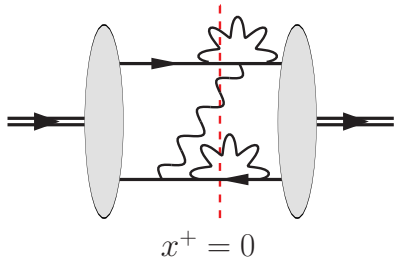
- Lorentz transformation: $ct' = \gamma_V(ct + \beta_V z) \overset{V\to\infty}{\to} \gamma_V x^+$
- Feynman's parton model: partons are free as time dilation beats interactions at a scale $\tau_{\rm QCD} \sim \Lambda_{\rm QCD}^{-1}$
- Renewed interests in efforts to extract parton distributions from Euclidean QFTs, e.g. LaMET, and interpolating between equal-time and light-front quantization [X.d. Ji, PRL '13; C.R. Ji '18]

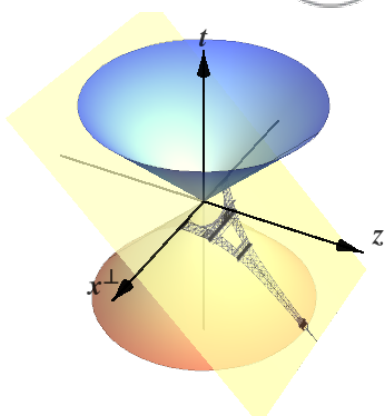


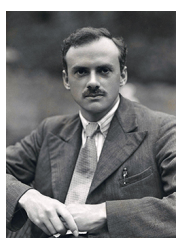
Hadron photography

- Due to the finiteness of the speed of light, the light-front way is the natural way to see things.
- Dirac's front-form quantization: initial hyper-surface where you can specify the canonical commutation relation and define the probability amplitudes (wave functions).
- Hadron is not moving at an infinite momentum! It is just the way how we see it.

Particle can be at rest in light-front dynamics: $P^+ = M, \vec{P}_\perp = 0$.







Scalar theory

The Lagrangian of the system is,

$$\mathscr{L} = \partial_\mu \chi^\dagger \partial^\mu \chi - m_\chi^2 \chi^\dagger \chi + \frac{1}{2}\partial_\mu \varphi \partial^\mu \varphi - \frac{1}{2} m_\varphi^2 \varphi^2 + g \chi^\dagger \chi \varphi. \tag{8}$$

The corresponding light-front Hamiltonian is,

$$P^- = \int \mathrm{d}^3 x \left\{ \chi^\dagger \left[(i\nabla_\perp)^2 + m_\chi^2 \right] \chi + \frac{1}{2} \varphi \left[(i\nabla_\perp)^2 + m_\varphi^2 \right] \varphi - g \chi^\dagger \chi \varphi \right\} \tag{9}$$

At the initial time $x^+ = 0$, the field operators can be expanded as,

$$\chi(x) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p^+} \left[b(p) e^{ip\cdot x} + d^\dagger(p) e^{-ip\cdot x} \right], \tag{10}$$

$$\varphi(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k^+} \left[a(k) e^{ik\cdot x} + a^\dagger(k) e^{-ik\cdot x} \right]. \tag{11}$$

Discussion on Oct. 22, 2021

Second quantization

Wave function of two free indistinguishable particles:

$$\langle x_1, x_2 | \alpha\beta \rangle \equiv \psi_{\alpha\beta}(x_1, x_2) = \psi_\alpha(x_1)\psi_\beta(x_2) \pm \psi_\alpha(x_2)\psi_\beta(x_1)$$

α, β are quantum numbers. The sign is determined by particle statistics. In the general n-body case,

$$\langle x_1, x_2, \cdots, x_n | \alpha_1, \alpha_2, \cdots, \alpha_n \rangle = \sum_{\sigma \in S_n} (-1)^{\mathrm{Sgn}(\sigma)} \psi_{\alpha_1}(x_{\sigma_1})\psi_{\alpha_2}(x_{\sigma_2}) \cdots \psi_{\alpha_n}(x_{\sigma_n})$$

Here S_n is the permutation group. $\{\sigma_1, \sigma_2, \cdots, \sigma_n\} = \sigma\{x_1, x_2, \cdots, x_n\}$ is a permutation of $\{x_1, x_2, \cdots, x_n\}$.

Dirac introduced the creation and annihilation operators to simplify the (anti-)symmetrization.

$$|\alpha_1, \alpha_2, \cdots, \alpha_n\rangle \equiv N a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \cdots a^\dagger_{\alpha_n} |0\rangle.$$

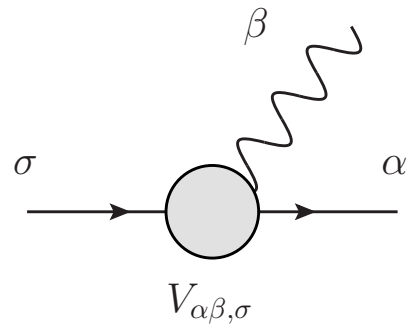
Here, the operators satisfies

$$a_\alpha a^\dagger_\beta \pm a^\dagger_\alpha a_\beta \equiv \left[a_\alpha, a^\dagger_\beta\right]_\pm = \delta_{\alpha\beta}.$$

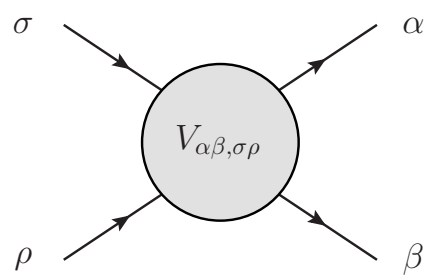
Diagrammaticsm I

Feynman diagrams for generic interactions

$$V = \sum_{\alpha,\beta,\sigma} V_{\alpha\beta,\sigma} b_\alpha^\dagger a_\beta^\dagger b_\sigma$$



$$V = \sum_{\alpha,\beta,\sigma\rho} V_{\alpha\beta,\sigma\rho} b_\alpha^\dagger b_\beta^\dagger b_\sigma b_\rho$$

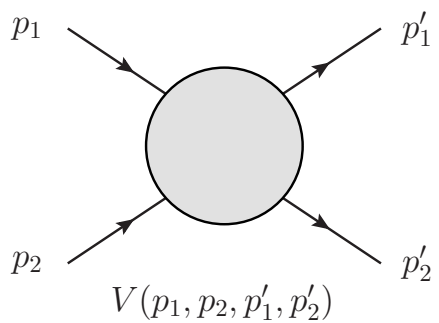


Exercise 1: write down Feynman rules for $H_0 = \sum_{\alpha,\beta} \left(\epsilon_\alpha \delta_{\alpha\beta} + u_{\alpha\beta}\right) c_\alpha^\dagger c_\beta$

Diagrammaticsm II: momentum representation

In momentum space, 3-momentum conservation is manifest. It is understood that each tensor block is associated with a Dirac delta $\delta^3(p_i - p_f)$

$$V = \int \frac{\mathrm{d}^3 p_1}{(2\pi)^3 2p_1^+} \frac{\mathrm{d}^3 p_2}{(2\pi)^3 2p_2^+} \frac{\mathrm{d}^3 p_1'}{(2\pi)^3 2p_1'^+} \frac{\mathrm{d}^3 p_2'}{(2\pi)^3 2p_2'^+}$$
$$\times 2P^+(2\pi)^3\delta^3(p_1 + p_2 - p_1' - p_2')V(p_1, p_2, p_1', p_2')$$
$$\times b^\dagger(p_2')b^\dagger(p_1')b(p_1)b(p_2)$$



N.B. in harmonic oscillator basis, angular momentum is conserved.

Diagrammaticsm III: local interactions

Local interactions:

$$H_{\text{int}}(t) = \int \mathrm{d}^3 x \, \mathcal{H}_{\text{int}}(x)$$

- Local interactions can be built from local fields, e.g.,

$$\psi(x) = \sum_\sigma \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p^+} \left[u_\sigma(p) e^{ip\cdot x} b_\sigma(p) + v_\sigma(p) e^{-ip\cdot x} d^\dagger_\sigma(p) \right]$$

  Covariance is easily maintained.

- Why local interactions are important in relativistic QFTs?

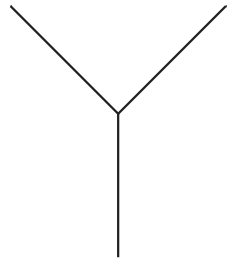
$$\left[\mathcal{H}_{\text{int}}(x), \mathcal{H}_{\text{int}}(x') \right] = 0, \quad \forall (x - x')^2 < 0.$$

  Physically, causality requires spacelike separated events do not causally affect each other via interaction.

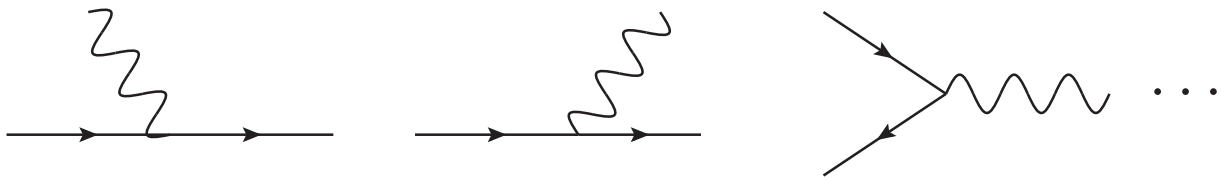
- Local interactions can be represented by (contact) vertices

Diagrammaticsm III: local interactions

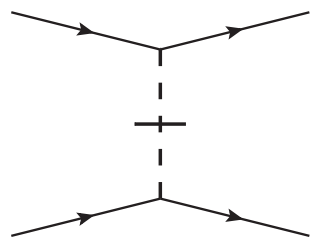
$$V = \int \mathrm{d}^3 x \left(\varphi(x)\right)^3$$



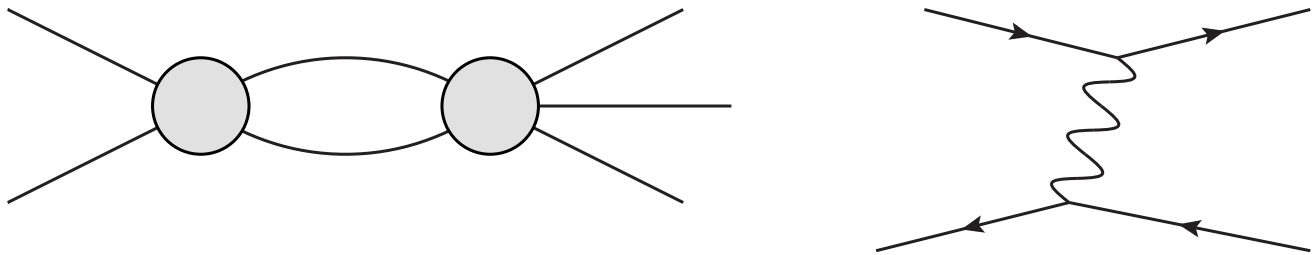
$$V = \int \mathrm{d}^3 x \overline{\psi}(x) \gamma^\mu \psi(x) A_\mu(x)$$



$$V = \int \mathrm{d}^3 x \mathrm{d}^3 x' n(x) U(|\vec{x} - \vec{x}'|) n(x'), \quad \left[n(x) \equiv \psi^\dagger(x)\psi(x)\right]$$



Diagrammaticsm IV: tensor contractions



Scattering I: Dyson formula

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle. \quad \Rightarrow |\psi(t_f)\rangle \sim e^{-iHt}|\psi(t_i)\rangle$$

Dyson formula: formal solution of Schrödinger equation, $|\psi(t_f)\rangle \equiv U(t_f,t_i)|\psi(t_i)\rangle$

$$U(t_f,t_i) = \mathcal{T}\exp\Big\{-i\int_{t_i}^{t_f} \mathrm{d}t H(t)\Big\},$$

$$= 1 - i\int_{t_i}^{t_f} \mathrm{d}t H(t) + \frac{(-i)^2}{2!}\int_{t_i}^{t_f} \mathrm{d}t_1\mathrm{d}t_2 \mathcal{T}\big\{H(t_1)H(t_2)\big\} + \cdots$$

Here, the time-ordering operation is defined as,

$$\mathcal{T}\big\{H(t_1)H(t_2)\big\} = \theta(t_1-t_2)H(t_1)H(t_2) + \theta(t_2-t_1)H(t_2)H(t_1)$$

Therefore,

$$\frac{1}{2!}\int_{t_i}^{t_f} \mathrm{d}t_1\mathrm{d}t_2 \mathcal{T}\big\{H(t_1)H(t_2)\big\} = \int_{t_i}^{t_f} \mathrm{d}t_1\mathrm{d}t_2 \theta(t_1-t_2)H(t_1)H(t_2)$$

Scattering II: S-matrix

Scattering amplitude and S-matrix:

$$\langle \psi(t_f \to \infty) | \psi(t_i \to -\infty) \rangle \equiv \langle \phi_\alpha | S | \phi_\beta \rangle$$

where $|\psi(t_i)\rangle \to e^{-iH_0 t_i} |\phi_\beta\rangle$ as $t_i \to -\infty$, $|\psi(t_f)\rangle \to e^{-iH_0 t_f} |\phi_\alpha\rangle$ as $t_f \to +\infty$.
The transition amplitude $i\mathcal{M}_{\alpha\beta} = \langle \phi_\alpha | S - 1 | \phi_\beta \rangle$.

Formal solution in the interaction picture:

$$\begin{aligned} S &= U_I(+\infty, -\infty) \\ &= \mathcal{T} \exp\left\{ -i \int \mathrm{d}t H_I(t) \right\} \\ &= 1 - i \int \mathrm{d}t H_I(t) + (-i)^2 \int \mathrm{d}t_1 \mathrm{d}t_2 \theta(t_1 - t_2) H_I(t_1) H_I(t_2) + \cdots \end{aligned}$$

Consider the leading order (LO) term

$$\int \mathrm{d}t H_I(t) = \int \mathrm{d}^4 x \mathcal{H}_I(x) = \widetilde{\mathcal{H}_I}(0)$$

where

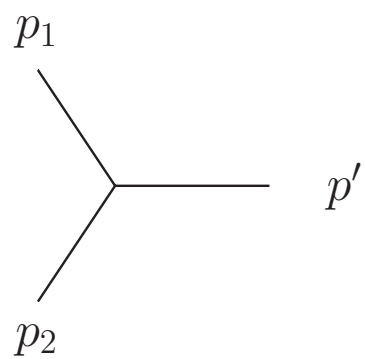
$$\widetilde{\mathcal{H}_I}(p) = \int \mathrm{d}^4 x \, e^{ip\cdot x} \mathcal{H}_I(x)$$

Scattering III: perturbation theory

Example: ϕ^3 theory, $\mathcal{H} = g\varphi^3$

$$\widetilde{\mathcal{H}_I}(0) = g \int \frac{\mathrm{d}^3 p_1}{(2\pi)^3 2p_1^0} \frac{\mathrm{d}^3 p_2}{(2\pi)^3 2p_2^0} \int \frac{\mathrm{d}^3 p_3}{(2\pi)^3 2p_3^0} \times (2\pi)^4 \delta^4(p_1 - p_2 - p_3) a^\dagger(p_1) a(p_2) a(p_3) + \cdots$$

$$i\mathcal{M}^{(1)}(p_1 + p_2 \to p') = \langle p' | \widetilde{\mathcal{H}_I}(0) | p_1 p_2 \rangle = (2\pi)^4 \delta^4(p_1 + p_2 - p') g$$



Scattering III: perturbation theory

For the next-to-leading order (NLO) term, consider the Fourier transform of the θ-function:

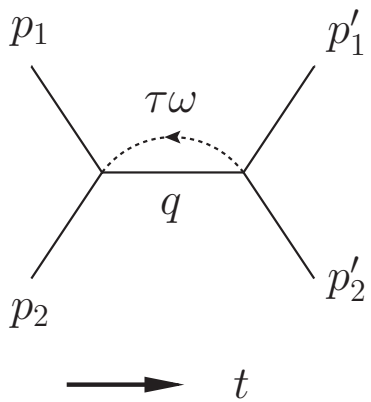
$$\theta(t) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} \mathrm{d}\tau \frac{e^{i\tau t}}{\tau - i\epsilon}$$

Then,

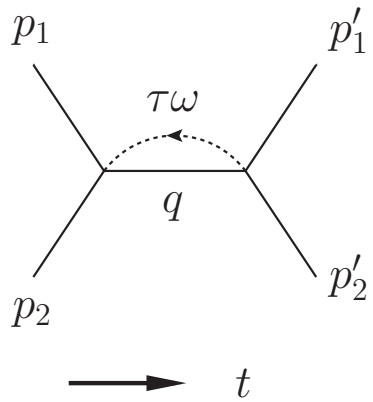
$$\int \mathrm{d}t_1 \mathrm{d}t_2 \theta(t_1 - t_2) H_I(t_1) H_I(t_2) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} \frac{\mathrm{d}\tau}{\tau - i\epsilon} \widetilde{\mathcal{H}}_I(\tau\omega)\widetilde{\mathcal{H}}_I(-\tau\omega)$$

Here ω^μ is a 4-vector pointing to the time direction. For instant form $\omega^\mu = (1, \vec{0})$. For front form $\omega^\mu = (\omega^-, \omega^+, \vec{\omega}_\perp) = (2, 0, 0_\perp)$.

$$i\mathcal{M}^{(2)}(p_1 + p_2 \to p_1' + p_2') = \frac{-g^2}{2\pi i}\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{\omega - i\epsilon} \langle p_1 p_2 | \widetilde{\mathcal{H}}_I(\tau\omega)\widetilde{\mathcal{H}}_I(-\tau\omega) | p_1' p_2' \rangle$$



Scattering III: perturbation theory



- Energy is not conserved at each vertex and τ is the off-shell energy.
- For each internal line, there is an energy denominator $1/(\tau - i\epsilon)$.
- Total 4-momentum is conserved $p_i = p_f$.
- Diagrams are time ordered

Scattering III: Feynman rules

1. Arbitrary label by a number the vertices in the Feynman graph of order n. Orientate continuous lines (the lines of physical particles) in the direction from the smaller to the larger number. Initial particles are oriented as incoming into a graph, and final particles as outgoing. Connect by a directed dashed line (the spurion line) the vertices in the order of decreasing numbers. Diagrams in which there are vertices with all incoming or outgoing particle lines (vacuum vertices, as indicated in Fig. 2) can be omitted. Associate with each continuous line a corresponding four-momentum, and with each jth spurion line a four-momentum $\omega\tau_j$.
2. To each internal continuous line with four-momentum k, associate the propagator $\theta(\omega \cdot k)\delta(k^2 - m^2)$, and to each internal dashed line with four-momentum $\omega\tau_j$ the factor $1/(\tau_j - \mathrm{i}\varepsilon)$.
3. Associate with each vertex the coupling constant g. All the four-momenta at the vertex, *including the spurion momenta*, satisfy the conservation law, i.e., the sum of incoming momenta is equal to the sum of outgoing momenta.
4. Integrate (with $\mathrm{d}^4k/(2\pi)^3$) over those four-momenta of the internal particles which remain unfixed after taking into account the conservation laws, and over all τ_j for the spurion lines from $-\infty$ to ∞.
5. Repeat the procedure described in 1–4 for all $n!$ possible numberings of the vertices.

J. Carbonell et al., Physical Reports, **300** (1998) 215-347.

Diagrammatics for Schrödinger equation

$$H|\psi_n\rangle = E_n|\psi_n\rangle \tag{12}$$

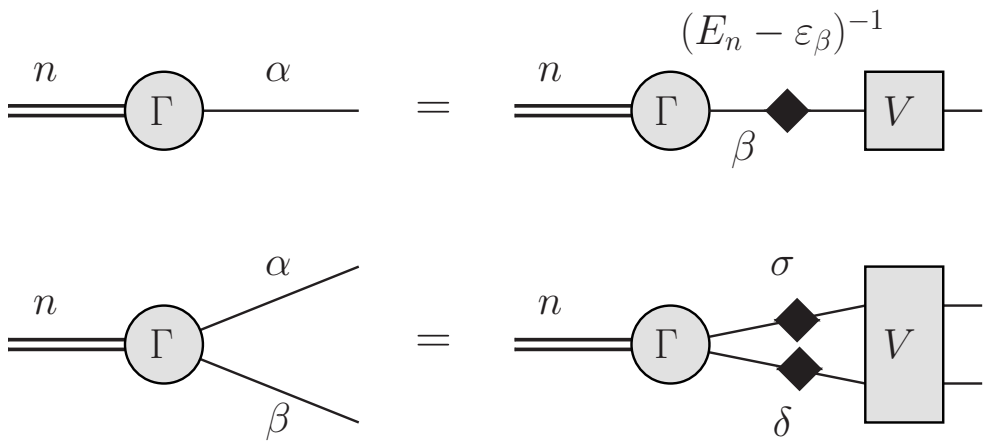
$$\Rightarrow \quad (H_0 + V)|\psi_n\rangle = E_n|\psi_n\rangle \qquad (H_0 \text{ is an ``simple'' Hamiltonian})$$

$$\Rightarrow \quad V|\psi_n\rangle = (E_n - H_0)|\psi_n\rangle$$

$$\Rightarrow \quad V(E_n + i\epsilon - H_0)^{-1}|\Gamma_n\rangle = |\Gamma_n\rangle \qquad |\Gamma_n\rangle \equiv (E_n - H_0)|\psi_n\rangle$$

$$\Rightarrow \quad \sum_\beta \frac{\langle\alpha|V|\beta\rangle\langle\beta|\Gamma_n\rangle}{E_n + i\epsilon - \varepsilon_\beta} = \langle\alpha|\Gamma_n\rangle \qquad \langle\alpha|H_0|\beta\rangle = \varepsilon_\alpha\delta_{\alpha\beta}$$

$$\Rightarrow \quad \sum_\beta \frac{V_{\alpha\beta}\Gamma_{\beta n}}{E_n + i\epsilon - \varepsilon_\beta} = \Gamma_{\alpha n} \qquad V_{\alpha\beta} \equiv \langle\alpha|V|\beta\rangle, \Gamma_{\alpha n} \equiv \langle\alpha|\Gamma_n\rangle$$



$$\Gamma^{(n+1)} = VG_0\Gamma^{(n)} \; (G_0 = (E - H_0)^{-1})$$

Lippmann-Schwinger equation

How to generalize the results to the non-perturbative regime?

- Vertex diagrams $V_{\alpha\beta} \equiv \langle \phi_\alpha | V | \phi_\beta \rangle$ here $|\phi_\alpha\rangle = c_\alpha^\dagger |0\rangle$ is the free Fock state and $H_0 |\phi_\alpha\rangle = \varepsilon_\alpha |\phi_\alpha\rangle$
- Lippmann-Schwinger equation:

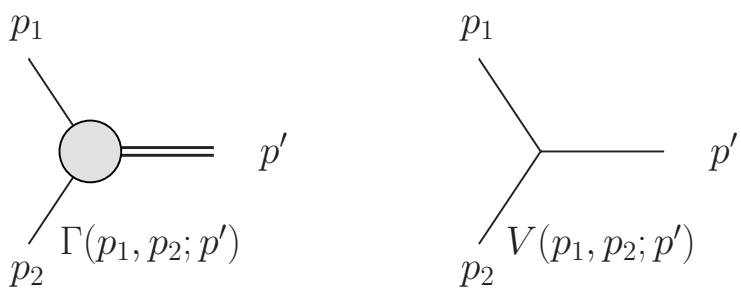
$$H|\psi_\alpha\rangle = E_\alpha |\psi_\alpha\rangle \;\Rightarrow\; |\psi_\alpha\rangle = |\phi_\alpha\rangle + G_0^{-1} V |\psi_\alpha\rangle,$$

  $G_0 = (E_\alpha + i\epsilon - H_0)^{-1}$ is the (free) resolvent operator.

- T-matrix:

$$\Gamma_{\alpha\beta} \equiv \langle \phi_\alpha | T | \phi_\beta \rangle \equiv \langle \phi_\alpha | V | \psi_\beta \rangle = (E_\beta + i\epsilon - \varepsilon_\alpha) \langle \phi_\alpha | \psi_\beta \rangle$$

  T-matrix consists of composite vertices



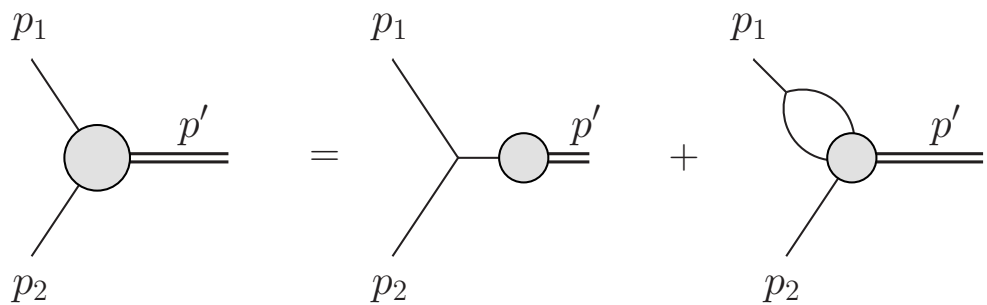
Diagrammaticsm IV: Kadyshevsky equation

T-matrix satisfies an integral equation:

$$\sum_{\{\beta_i\}} \frac{V_{\alpha,\{\beta_i\}}\Gamma_{\{\beta_i\},n}}{E_n + i\epsilon - \varepsilon_{\{\beta_i\}}} = \Gamma_{\alpha,n}$$

where $V_{\alpha,\{\beta_i\}} = \langle\alpha|V|\{\beta_i\}\rangle$, $\Gamma_{\alpha,\{\beta_i\}} = \langle\alpha|T|\{\beta_i\}\rangle$, and, $\sum_{\{\beta_i\}} |\{\beta_i\}\rangle\langle\{\beta_i\}| = 1$ is the complete Fock space basis. The the total energy $\varepsilon_{\{\beta_i\}}$,

$$\varepsilon_{\{\beta_i\}} = \begin{cases} \sum_i \sqrt{\vec{p}_i^2 + m_i} & \text{instant form,} \\ \sum_i \frac{\vec{p}_{i\perp}^2 + m_i^2}{p_i^+}, & \text{front form} \end{cases}$$



We can generalize the Feynman rules in perturbation theory to non-perturbative theory by incorporating the T-matrix elements.

References

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2. J. Carbonell et al., Physical Reports, **300** (1998) 215-347. Chapter 2.

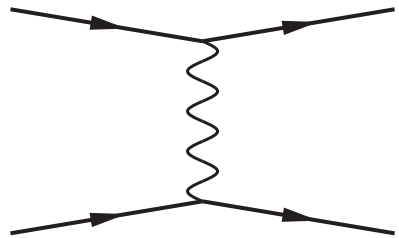
3. S.J. Brodsky et al., Physical Reports, **301** (1998) 299-486. Sect. 2.8-3.4

4. M.E. Peskin and D.V. Schroeder, An introduction to quantum field theory, Chapter 4. Westview Press (1995). ISBN: 0-201-50397-2.

Discussion on Oct. 29, 2021

Scalar Yukawa theory

As a concrete example, let us consider a scalar theory consists of a charged scalar field $\chi(x)$ and a light neutral scalar $\varphi(x)$ interacting through the Yukawa coupling $\mathscr{L}_{\text{int}} = g\chi^\dagger\chi\varphi$.



The Lagrangian of the system is,

$$\mathscr{L} = \partial_\mu\chi^\dagger\partial^\mu\chi - m_\chi^2\chi^\dagger\chi + \frac{1}{2}\partial_\mu\varphi\partial^\mu\varphi - \frac{1}{2}m_\varphi^2\varphi^2 + g\chi^\dagger\chi\varphi.$$

Here m_χ and m_φ are the masses of the two species. We tentatively choose $m_\chi = 0.94\,\text{GeV}$ and $m_\varphi = 0.14\,\text{GeV}$. The theory thus describes the pion-nucleon interaction. The corresponding semiclassical nucleon-nucleon interaction is the Yukawa potential, $V_{NN}(r) = -\alpha\exp(-m_\varphi r)/r$, where $\alpha = g^2/16\pi m_\chi^2$.

Quantization

- What is quantization?

  The quantization of a dynamical system is to pick out the physical generalized coordinates q_i and generalized momenta p_i and to impose the appropriate commutation relations $\{q_i, p_j\} \rightarrow (i/\hbar)[q_i, p_j]$.

- Quantization of this theory on the light front $x^+ = 0$ involves constraint quantization.

  However, observe that the Lagrangian is similar to the Schrödinger field ($\dot{f} = \partial f/\partial x^+$)

$$\mathscr{L}_0 = \frac{1}{2}\left[\dot{\chi}^\dagger \partial^+ \chi + \partial^+ \chi^\dagger \dot{\chi}\right] - \nabla_\perp \chi^\dagger \cdot \nabla_\perp \chi - m_\chi^2 \chi^\dagger \chi$$

- Light-front Hamiltonian,

$$P^- = \int \mathrm{d}^3x \left\{\chi^\dagger\left[(i\nabla_\perp)^2 + m_\chi^2\right]\chi + \frac{1}{2}\varphi\left[(i\nabla_\perp)^2 + m_\varphi^2\right]\varphi - g\chi^\dagger\chi\varphi\right\}$$

$$\chi(x) = \int \frac{\mathrm{d}^3p}{(2\pi)^3 2p^+}\left[b(p)e^{ip\cdot x} + d^\dagger(p)e^{-ip\cdot x}\right],$$

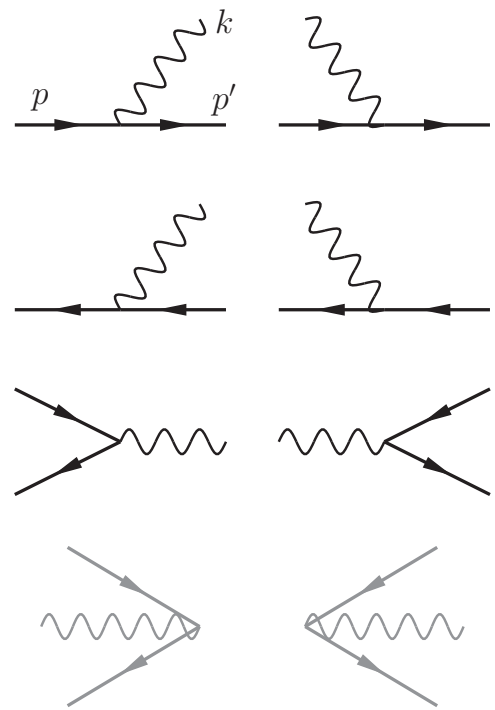
$$\varphi(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k^+}\left[a(k)e^{ik\cdot x} + a^\dagger(k)e^{-ik\cdot x}\right].$$

  where, $\left[c_i(p), c_j^\dagger(p')\right] = 2p^+(2\pi)^3\delta^3(p-p')\delta_{ij}$

Second quantization

Light-front Hamiltonian,

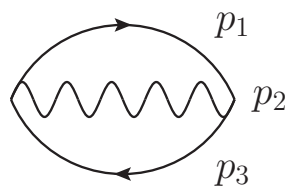
$$
\begin{aligned}
P^- &= \int \mathrm{d}^3x \left\{ \chi^\dagger \left[(i\nabla_\perp)^2 + m_\chi^2 \right] \chi + \frac{1}{2} \varphi \left[(i\nabla_\perp)^2 + m_\varphi^2 \right] \varphi - g \chi^\dagger \chi \varphi \right\} \\
&= \int \frac{\mathrm{d}^3p}{(2\pi)^3 2p^+} \frac{\vec{p}_\perp^{\,2} + m_\chi^2}{p^+} \left[b^\dagger(p) b(p) + d^\dagger(p) d(p) \right] \\
&+ \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k^+} \frac{\vec{k}_\perp^{\,2} + m_\varphi^2}{k^+} a^\dagger(k) a(k) \\
&- g \int \frac{\mathrm{d}^3p}{(2\pi)^3 2p^+} \frac{\mathrm{d}^3p'}{(2\pi)^3 2p'^+} \frac{\mathrm{d}^3k}{(2\pi)^3 2k^+} \\
&\quad \times \Big\{ b^\dagger(p) b(p') a(k) \, (2\pi)^3 \delta^3(p - p' - k) \\
&\quad + b^\dagger(p) b(p') a^\dagger(k) \, (2\pi)^3 \delta^3(p + k - p') \\
&\quad + d^\dagger(p) d(p') a(k) \, (2\pi)^3 \delta^3(p - p' - k) \\
&\quad + d^\dagger(p) d(p') a^\dagger(k) \, (2\pi)^3 \delta^3(p + k - p') \\
&\quad + b^\dagger(p) d^\dagger(p') a(k) \, (2\pi)^3 \delta^3(p + p' - k) \\
&\quad + b(p) d(p') a^\dagger(k) \, (2\pi)^3 \delta^3(k - p - p') \Big\}
\end{aligned}
$$



Light front variables

- For any 4-vector $V^\mu = (V^0, \vec{V})$, define the light-front components of V as, $V^\pm = V^0 \pm V^3$, $\vec{V}_\perp = (V^1, V^2)$.
- Scalar product: $V \cdot U = V^0 U^0 - \vec{V} \cdot \vec{U} = \frac{1}{2} V^+ U^- + \frac{1}{2} V^- U^+ - \vec{V}_\perp \cdot \vec{U}_\perp$. In particular, $V^2 = V^+ V^- - \vec{V}_\perp^2$.
- Coordinates: $x^+ = x^0 + x^3$ is light front time. x^- longitudinal coordinate, $\vec{x}_\perp$ transverse coordinate.

  Causality: for time-like separations $\Delta x^2 > 0$, $\theta(\Delta x^0) = \theta(\Delta x^+)$
- 4-momentum: $p \cdot x = \frac{1}{2} p^- x^+ + \frac{1}{2} p^+ x^- - \vec{p}_\perp \cdot \vec{x}_\perp$. Hence, p^- is light-front energy whereas p^+ is longitudinal momentum and $\vec{p}_\perp$ is transverse momentum.
- Dispersion relation: instant form $p^0 = \sqrt{\vec{p}^2 + m^2}$ vs front form $p^- = \frac{\vec{p}_\perp^2 + m^2}{p^+}$
  - No square root in front form dispersion relation!
  - Positivity of light-front energy $p^- \geq 0$ implies the positivity of longitudinal momentum $p^+ \geq 0$
  - Vacuum fluctuation is suppressed in light-front dynamics. $\mathcal{M} \propto \delta(\sum_i p_i^+) \to 0$



Light front kinematics

- Lorentz boosts:

$$
\begin{aligned}
p'^{-} &= e^{-\frac{1}{2}\beta^{-}}\left(p^{-} + \vec{\beta}_{\perp}^{2} p^{+} + 2\vec{\beta}_{\perp}\cdot\vec{p}_{\perp}\right), \\
p'^{+} &= e^{+\frac{1}{2}\beta^{-}} p^{+}, \\
\vec{p}'_{\perp} &= \vec{p}_{\perp} + p^{+}\vec{\beta}_{\perp}
\end{aligned}
$$

  Lorentz boosts in front form is similar to Galileo boosts, hence permitting simpler kinematics e.g. factorization of center of mass motion.

- Total/center-of-mass momentum:

$$
P^{+} = \sum_i p_i^{+}, \quad \vec{P}_{\perp} = \sum_i \vec{p}_{i\perp}
$$

- Relative momenta:

$$
x_i = p_i^{+}/P^{+}, \quad \vec{k}_{i\perp} = \vec{p}_{i\perp} - x_i \vec{P}_{\perp}.
$$

  Relative momenta are boost invariant.

- Lorentz invariant phase element:

$$
\begin{aligned}
\frac{\mathrm{d}^2 p}{(2\pi)^3 2p^0}\theta(p^0) &= \frac{\mathrm{d}p^{+}\mathrm{d}^2 p_{\perp}}{(2\pi)^3 2p^{+}}\theta(p^{+}) \\
2p^0\theta(p^0)\delta^3(p-p') &= 2p^{+}\theta(p^{+})\delta(p^{+}-p'^{+})\delta^2(p_{\perp}-p'_{\perp})
\end{aligned}
$$

Light front Schrödinger equation

Schrödinger equation of a particle with quantum number α,

$$\underline{P}^- |\psi_\alpha(p)\rangle = \frac{\vec{p}_\perp^2 + M_\alpha^2}{p^+} |\psi_\alpha(p)\rangle$$

Einstein equation:

$$\underline{\mathcal{M}}^2 |\psi_\alpha(p)\rangle = M_\alpha^2 |\psi_\alpha(p)\rangle$$

where $\underline{\mathcal{M}}^2 = p^+ \underline{P}^- - \vec{p}_\perp^2$ serves as the light-cone Hamiltonian. For example, $\underline{\mathcal{M}}^2 = \underline{\mathcal{M}}_0^2 + \underline{V}$, where $\underline{\mathcal{M}}_0^2 = p^+ \underline{P}_0^- - \vec{p}_\perp^2$, and $\underline{V} = p^+ \underline{P}_{\text{int}}^-$.

Light front wave functions

- Example: nucleon $|N\rangle = |\chi\rangle + |\chi\varphi\rangle + |\chi\varphi\varphi\rangle + \cdots$
- Light-front wave functions (LFWFs)s,

$$|\psi_N(p)\rangle = \Psi_\chi b^\dagger(p)|0\rangle + \int \frac{\mathrm{d}^3k_1}{(2\pi)^3 2k_1^+}\frac{\mathrm{d}^3k_2}{(2\pi)^3 2k_2^+} 2p^+(2\pi)^3\delta^3(k_1+k_2-p) \times \Psi_{\varphi\chi}(k_1,k_2;p)a^\dagger(k_1)b^\dagger(k_2)|0\rangle + \cdots$$

- LFWFs are boost invariant (frame-independent)

  They only depend on boost invariants $\Psi_n(k_1,k_2,\cdots,k_n;p) = \psi_n(x_1,\vec{\kappa}_{1\perp},\cdots,x_n,\vec{\kappa}_{n\perp})$ where $x_i \equiv k_i^+/p^+$, $\vec{\kappa}_{i\perp} = \vec{k}_{i\perp} - x_i\vec{p}_\perp$

  Momentum conservation implies, $\sum_i x_i = 1, \sum_i \vec{\kappa}_{i\perp} = 0$.

- Light-front kinematics:

$$\int \frac{\mathrm{d}^3k_1}{(2\pi)^3 2k_1^+}\frac{\mathrm{d}^3k_2}{(2\pi)^3 2k_2^+} 2p^+(2\pi)^3\delta^3(k_1+k_2-p) = \int \frac{\mathrm{d}x}{2x(1-x)}\frac{\mathrm{d}^2k_\perp}{(2\pi)^3}\psi(x,\vec{k}_\perp)$$

Diagrammatics

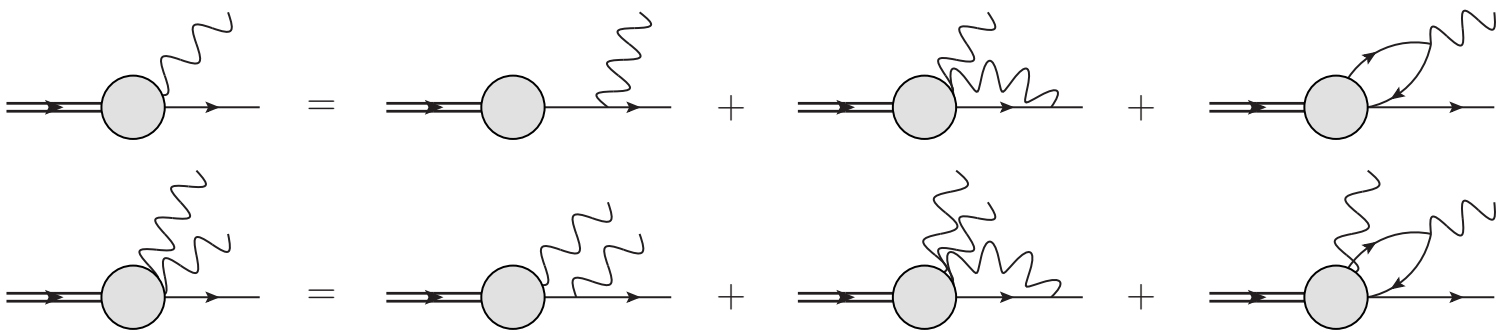
Recall T-matrix

$$\Gamma_n(k_1, k_2, \cdots, k_n; p) \equiv \langle k_1, k_2, \cdots, k_n | T | p \rangle = \langle k_1, k_2, \cdots, k_n | V | \psi(p) \rangle$$

Relation to LFWFs,

$$\psi_n(\{x_i, \vec{k}_{i\perp}\}) = \frac{\Gamma_n(\{x_i, \vec{k}_{i\perp}\})}{s_n - M^2},$$

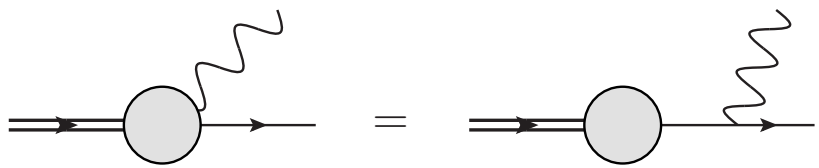
where $s_n = (p_1 + p_2 + \cdots + p_n)^2$ is the eigen-energy of the $\underline{\mathcal{M}}_0^2$ operator.



We get an infinite tower of coupled integral equations! Must do a truncation.

Diagrammatics

Two-body truncation:



$$\psi_2(x,\vec{k}_\perp) = \frac{g\psi_1}{\frac{\vec{k}_\perp^2+m_\varphi^2}{x} + \frac{\vec{k}_\perp^2+m_\chi^2}{1-x} - M^2}$$

where $2p^+(2\pi)^3\delta^3(p-k_1)\psi_1 = \langle k_1|\psi(p)\rangle$, and $\psi_1 = \langle 0|\chi(0)|\psi(p)\rangle \equiv \sqrt{Z_\chi}$ is a c-number.

Assignments

- *Exercise I:* Write down the integral equation for the diagrammatic equation in the first line.

- *Exercise II:* Show that the light-front kinetic energy,

$$\sum_i p_i^- = \frac{\vec{P}_\perp^2 + s_n}{P^+}$$

  where $P^+ = \sum_i p_i^+$, $\vec{P}_\perp = \sum_i \vec{p}_{i\perp}$ are the total light-front momenta. The effective mass $s_n \equiv (p_1 + p_2 + \cdots + p_n)^2$.

- *Exercise III:* Compute $s_n \equiv (p_1 + p_2 + \cdots + p_n)^2$ in instant form and in front form, where $p_i^2 = m_i^2$. Show that in front form, s_n only depends on the relative momenta $\{x_i, \vec{k}_{i\perp}\}$.

Assignments

- *Exercise IV:* Cluster decomposition:

Lemma *cluster decomposition of s*:

Let $(x_i, \boldsymbol{k}_{i\perp})$ be relative momenta $(i = 1, 2\cdots)$, i.e. $\sum_i x_i = 1$, $\sum_i \boldsymbol{k}_{i\perp} = 0$. Partition the system into two clusters A and B. Let $x_A = \sum_{i\in A} x_i, \boldsymbol{k}_{A\perp} = \sum_{i\in A} \boldsymbol{k}_{i\perp}, x_B = \sum_{i\in B} x_i, \boldsymbol{k}_{B\perp} = \sum_{i\in B} \boldsymbol{k}_{i\perp}$. Obviously, $\boldsymbol{k}_{A\perp} + \boldsymbol{k}_{B\perp} = 0$, $x_A + x_B = 1$.

Define new relative momenta with respect to the cluster: $\zeta_{iA} = x_i/x_A$, $\boldsymbol{\kappa}_{iA\perp} = \boldsymbol{k}_{i\perp} - \zeta_{iA}\boldsymbol{k}_{A\perp}$. $\zeta_{iB} = x_i/x_B$, $\boldsymbol{\kappa}_{iB\perp} = \boldsymbol{k}_{i\perp} - \zeta_{iB}\boldsymbol{k}_{B\perp}$. Introduce the invariant masses $s_A = \sum_{i\in A} \frac{\boldsymbol{\kappa}^2_{iA\perp}+m_i^2}{\zeta_{iA}}$, $s_B = \sum_{i\in B} \frac{\boldsymbol{\kappa}^2_{iB\perp}+m_i^2}{\zeta_{iB}}$.

Then, the total invariant mass squared $s \equiv s_{A+B} = \sum_i \frac{\boldsymbol{k}^2_{i\perp}+m_i^2}{x_i}$ can be written as,

$$\sum_i \frac{\boldsymbol{k}^2_{i\perp} + m_i^2}{x_i} = \frac{\boldsymbol{k}^2_{A\perp} + s_A}{x_A} + \frac{\boldsymbol{k}^2_{A\perp} + s_B}{1 - x_A} \tag{24}$$

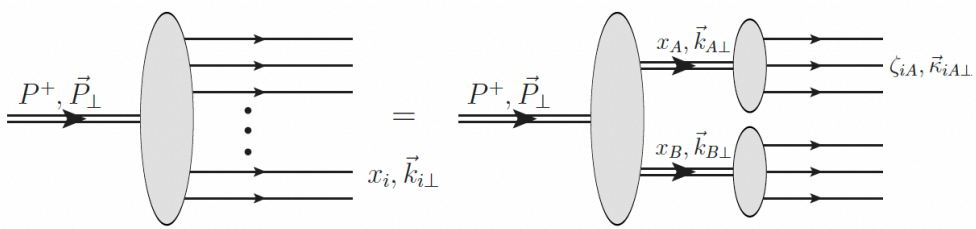


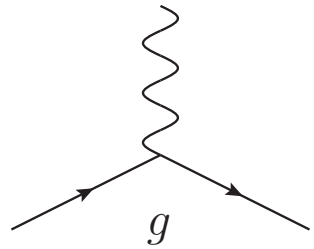
Figure 2: Cluster decomposition of the few-body invariant mass squared.

References

- V.A. Karmanov et al., Phys. Rev. D **94**, 096008 (2016)

Discussion on Nov. 12, 2021

Scalar Yukawa theory



The Lagrangian of the system is,

$$\mathscr{L} = \partial_\mu \chi^\dagger \partial^\mu \chi - m_\chi^2 \chi^\dagger \chi + \tfrac{1}{2}\partial_\mu \varphi \partial^\mu \varphi - \tfrac{1}{2} m_\varphi^2 \varphi^2 + g \chi^\dagger \chi \varphi.$$

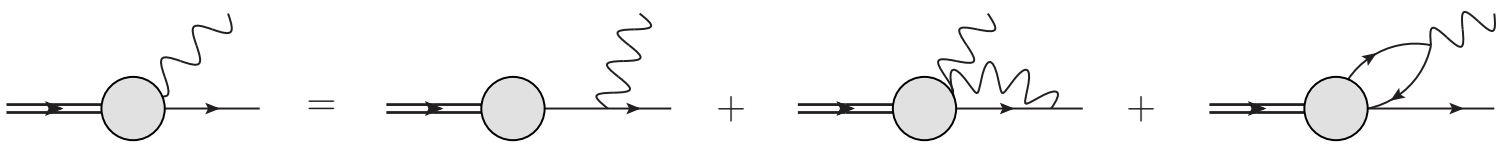
The light-front Hamiltonian,

$$P^- = \int \mathrm{d}^3 x \left\{ \chi^\dagger \left[(i\nabla_\perp)^2 + m_\chi^2 \right] \chi + \tfrac{1}{2} \varphi \left[(i\nabla_\perp)^2 + m_\varphi^2 \right] \varphi - g \chi^\dagger \chi \varphi \right\}$$

Light-front Schrödinger equation and Einstein equation,

$$\underline{P}^- |\psi_\alpha(p)\rangle = \frac{\vec{p}_\perp^{\,2} + M_\alpha^2}{p^+} |\psi_\alpha(p)\rangle \Rightarrow \underline{\mathcal{M}}^2 |\psi_\alpha(p)\rangle = M_\alpha^2 |\psi_\alpha(p)\rangle$$

Light-front wave function, T-matrix, and diagrammatic representation,



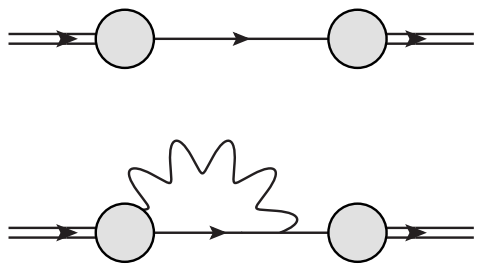
Renormalization: mass

All parameters appearing in the Lagrangian are bare parameters, not directly observables. Why? Because fields are not particles!

$$\mathscr{L} = \partial_\mu \chi_0^\dagger \partial^\mu \chi_0 - m_{\chi 0}^2 \chi_0^\dagger \chi_0 + \tfrac{1}{2}\partial_\mu \varphi_0 \partial^\mu \varphi_0 - \tfrac{1}{2} m_{\varphi 0}^2 \varphi_0^2 + g_0 \chi_0^\dagger \chi_0 \varphi_0.$$

They only coincide with the physical parameters if there is no interaction (or protected by symmetries).

Example 1: particle mass $m \neq m_0$ due to quantum fluctuation



$$M^2 = \langle \psi | \mathcal{M}^2 | \psi \rangle = m_0^2 \langle \chi | \chi \rangle - \int \mathrm{d}^3 x \langle \chi | g_0 \chi^\dagger \chi \varphi | \chi \varphi \rangle + \cdots$$

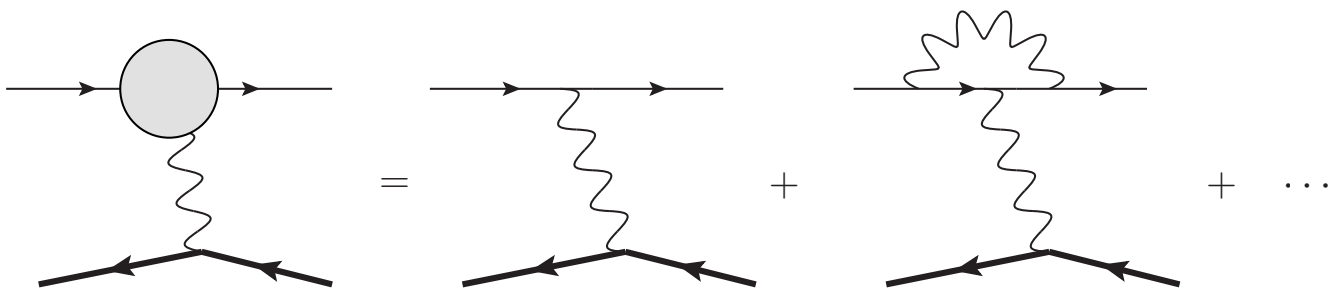
Renormalization: coupling constant

All parameters appearing in the Lagrangian are bare parameters, not directly observables. Why? Because fields are not particles!

$$\mathscr{L} = \partial_\mu \chi_0^\dagger \partial^\mu \chi_0 - m_{\chi 0}^2 \chi_0^\dagger \chi_0 + \tfrac{1}{2}\partial_\mu \varphi_0 \partial^\mu \varphi_0 - \tfrac{1}{2} m_{\varphi 0}^2 \varphi_0^2 + g_0 \chi_0^\dagger \chi_0 \varphi_0.$$

They only coincide with the physical parameters if there is no interaction (or protected by symmetries).

Example 2: coupling constant $g \neq g_0$ due to quantum fluctuation



$$i\mathcal{M} = \frac{iV_2(x, k_\perp)}{q^2 - \mu^2 + i\epsilon} = \frac{ig_0}{q^2 - \mu^2 + i\epsilon} + \cdots \overset{q^2 \to \mu^2}{\sim} \frac{ig}{q^2 - \mu^2 + i\epsilon}$$

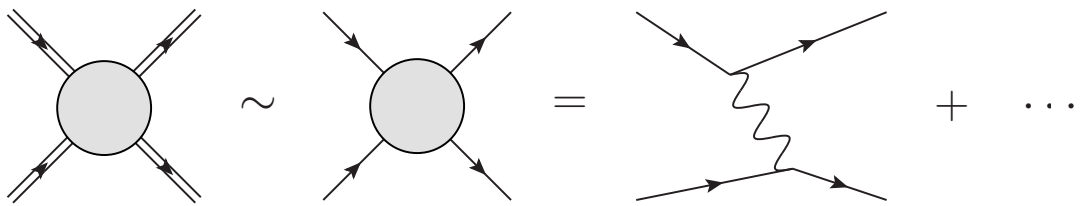
Renormalization: field strength

All parameters appearing in the Lagrangian are bare parameters, not directly observables. Why? Because fields are not particles!

$$\mathscr{L} = \partial_\mu \chi_0^\dagger \partial^\mu \chi_0 - m_{\chi 0}^2 \chi_0^\dagger \chi_0 + \tfrac{1}{2}\partial_\mu \varphi_0 \partial^\mu \varphi_0 - \tfrac{1}{2} m_{\varphi 0}^2 \varphi_0^2 + g_0 \chi_0^\dagger \chi_0 \varphi_0.$$

They only coincide with the physical parameters if there is no interaction (or protected by symmetries).

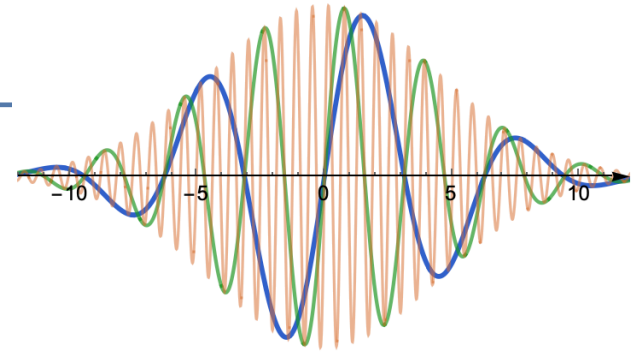
Example 3: particle scattering vs field scattering



$$|\psi(p)\rangle = \sqrt{Z} b^\dagger(p)|0\rangle + \int [\mathrm{d}x\, \mathrm{d}^2 k_\perp] \psi_2(x, \vec{k}_\perp) b^\dagger(p_1) a^\dagger(p_2)|0\rangle + \cdots$$

$$\neq b^\dagger(p)|0\rangle$$

让子弹飞一会儿



Lemma (Riemann–Lebesgue)

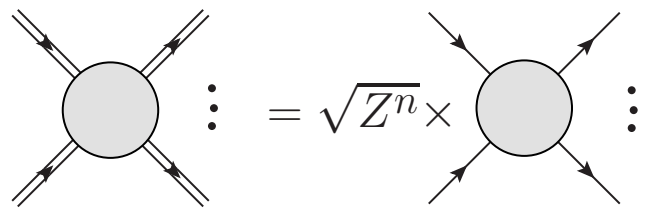
If $f(x) \in L^1(\mathbb{R}^n)$, *then as* $|z| \to \infty$,

$$\int \mathrm{d}^n x\, f(x) e^{-iz\cdot x} \to 0.$$

Create asymptotic states using Riemann-Lebesgue lemma:

$$e^{-\frac{i}{2}\underline{P}^- x^+}\underline{\chi}(x)|0\rangle = \sum_\alpha \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p^+} e^{-ip_\alpha\cdot x}|\psi_\alpha(p)\rangle\langle\psi_\alpha(p)|\underline{\chi}(0)|0\rangle$$

$$\xrightarrow{x^+\to\infty} e^{-ip_0\cdot x}|\psi_0(p)\rangle\sqrt{Z}$$



alternatively, $\chi_0 \to \chi = \chi_0/\sqrt{Z}$

Field redefinition/renormalization

Original Lagrangian,

$$\mathscr{L}_{\mathrm{I}} = -\chi_0^\dagger\left[\partial^2 + m_{\chi 0}^2\right]\chi_0 - \tfrac{1}{2}\varphi_0\left[\partial^2 + \tfrac{1}{2}m_{\varphi 0}^2\right]\varphi_0 + g_0\chi_0^\dagger\chi_0\varphi_0.$$

Form II:

$$\mathscr{L}_{\mathrm{II}} = -\chi_0^\dagger\left[\partial^2 + m_\chi^2\right]\chi_0 - \tfrac{1}{2}\varphi_0\left[\partial^2 + m_\varphi^2\right]\varphi_0 + g_0\chi_0^\dagger\chi_0\varphi_0 - \delta m_\chi^2\chi_0^\dagger\chi_0 - \tfrac{1}{2}\delta m_\varphi^2\varphi_0^2$$

$\delta m^2 = m_0^2 - m^2$, are called the mass counterterms.

Form III:

$$\mathscr{L}_{\mathrm{III}} = -\chi^\dagger\left[\partial^2 + m_\chi^2\right]\chi - \tfrac{1}{2}\varphi\left[\partial^2 + m_\varphi^2\right]\varphi + g\chi^\dagger\chi\varphi - (\delta Z_\chi\partial^2 + \delta m_\chi^2)\chi^\dagger\chi - \tfrac{1}{2}(\delta Z_\varphi\partial^2 + \delta m_\varphi^2)\varphi^2 + \delta Z_g g\chi^\dagger\chi\varphi$$

Field redefinitions: $\chi = \chi_0/\sqrt{Z_\chi}$, $\varphi = \varphi_0/\sqrt{Z_\varphi}$, $g = g_0 Z_\chi\sqrt{Z_\varphi}/Z_g$
Counterterms: $\delta m^2 = m^2 - Zm_0^2$, $\delta Z = Z - 1$,

$$\mathscr{L}_{\mathrm{I}} = \mathscr{L}_{\mathrm{II}} = \mathscr{L}_{\mathrm{III}} = \cdots$$

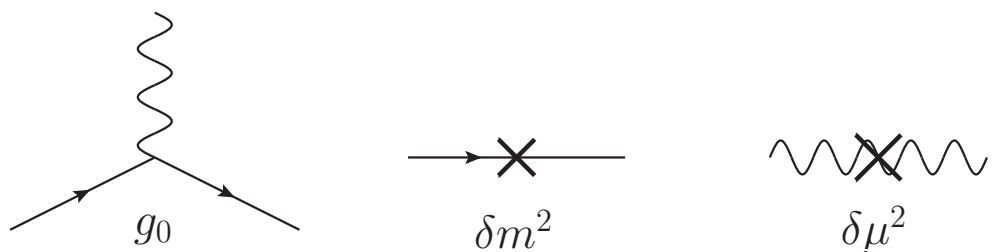
Redefined/renormalized vertices

It turns out, in the Hamiltonian formalism, one of the the convenient form is,

$$\mathscr{L} = -\chi_0^\dagger \left[\partial^2 + m_\chi^2\right]\chi_0 - \tfrac{1}{2}\varphi_0\left[\partial^2 + m_\varphi^2\right]\varphi_0 + g_0\chi_0^\dagger\chi_0\varphi_0 - \delta m_\chi^2\chi_0^\dagger\chi_0 - \tfrac{1}{2}\delta m_\varphi^2\varphi_0^2$$

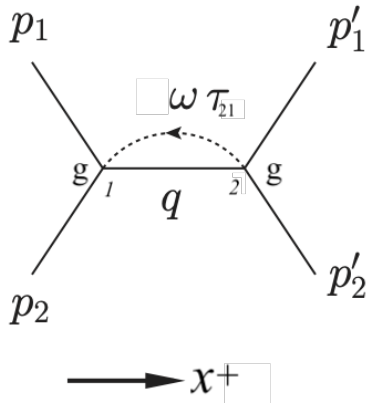
Drop the subscripts to simplify the notations,

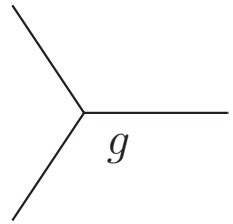
$$\mathscr{L} = \mathscr{L}_0 + \mathscr{L}_{\text{int}} = -\chi^\dagger\left[\partial^2 + m^2\right]\chi - \tfrac{1}{2}\varphi\left[\partial^2 + \mu^2\right]\varphi + g_0\chi^\dagger\chi\varphi - \delta m^2\chi^\dagger\chi - \tfrac{1}{2}\delta\mu^2\varphi^2$$



Discussion on Nov. 26, 2021

Feynman rules (scalar theory)

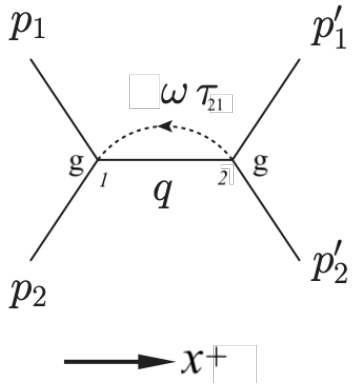




How to draw time-ordered diagrams:

1. Draw a connected time-ordered graph for designated initial and final states. The vertices are those allowed by the interactions;
2. Associate each line an appropriate 4 momentum;
3. Associate each vertex a coupling provided by the vertex rule of the theory;
4. Connect the vertices using dashed lines in the order against the direction of the time;
5. Associate each dashed line a spurious 4-momentum $\omega\tau_{ij}$, where ω is a null vector in the light cone direction. τ_{ij} is a number connecting the vertex i to j;
6. If the initial or final state is also off-shell, continuate the spurious line to the off-shell initial or final state, and associate a spurious 4-momentum $\omega\tau_i$ or $\omega\tau_f$;

Feynman rules (scalar theory)

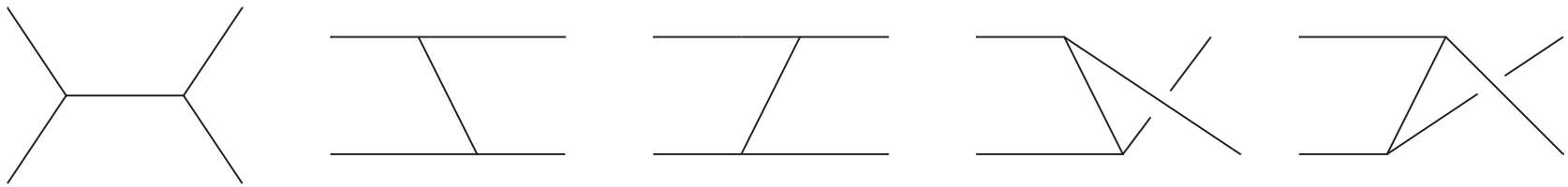


$$S_{fi} = \int \frac{\mathrm{d}^4 q}{(2\pi)^4} 2\pi\delta(q^2-\mu^2) \int \frac{\mathrm{d}\tau}{2\pi} \frac{1}{\tau - i\epsilon}$$
$$\times g(2\pi)^4\delta^4(p_1+p_2+\omega\tau-q) g(2\pi)^4\delta^4(q-p_1'-p_2'-\omega\tau)$$
$$= \frac{g^2}{(p_1+p_2)^2-\mu^2}(2\pi)^4\delta^4(p_1+p_2-p_1'-p_2')$$

How to translate the diagrams to expressions:

1. Each internal line with 4-momentum p_i contributes to a factor
$$\int \frac{\mathrm{d}^4 p_i}{(2\pi)^4}(2\pi)\delta(p_i^2-m_i^2) = \int \frac{\mathrm{d}^3 p_i}{(2\pi)^3 2p_i^+};$$
2. Each internal spurious line with 4-momentum $\omega\tau_{ij}$ contributes to a factor
$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}\tau_{ij}}{2\pi} \frac{1}{\tau_{ij}-i\epsilon}$$
3. Each vertex contributes to a factor specified by vertex rules (including T-matrix);
4. Each vertex contributes to the factor associated with the vertex and a 4-momentum conservation including the spurious momenta
$$(2\pi)^4\delta^4\Big(\sum_{i\in \text{in}} p_i + \omega\tau_i - \sum_{j\in\text{out}} p_j - \omega\tau_j\Big)$$

Feynman rules (scalar theory)

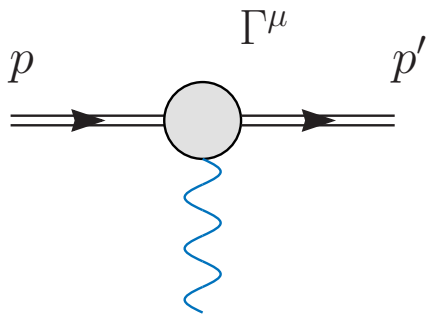


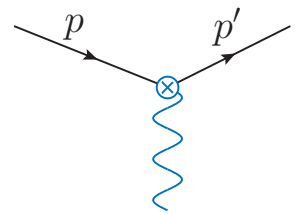
How to compute the S-matrix element:

1. Find and compute all topologically distinct time-ordered diagrams G with the same initial and final states.
2. The total S-matrix element is the superposition of all these diagrams listed above.

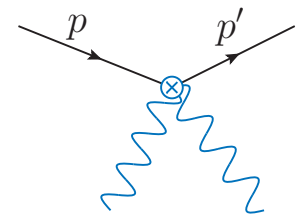
$$S_{fi} = \sum_{g \in G} S_{fi}^{(g)}$$

Example: electromagnetic vertex





$e(p+p')^\mu \epsilon_\mu$



$e^2 \epsilon_1 \cdot \epsilon_2$

$$\mathcal{M} = \int \mathrm{d}^4 x e^{iq\cdot x} \epsilon_\mu(q,\lambda) \langle p|J^\mu(x)|p'\rangle = (2\pi)^4 \delta^4(p+q-p')\epsilon_\mu(q,\lambda)\langle p|J^\mu(0)|p'\rangle$$

Lorentz decomposition of the hadronic matrix element:

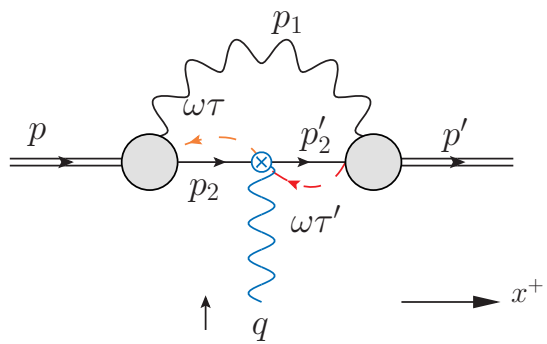
$$\Gamma^\mu \equiv \langle p|J^\mu(0)|p'\rangle = (p+p')^\mu F(q^2)$$

Interaction vertex: minimal coupling $\partial^\mu \to \partial^\mu - ie\mathcal{A}^\mu \equiv D^\mu$

$$\partial_\mu \chi^\dagger \partial^\mu \chi \;\to\; D_\mu \chi^\dagger D^\mu \chi = \partial_\mu \chi^\dagger \partial^\mu \chi - eA^\mu \left[i\partial^\mu \chi^\dagger \chi A^\mu - \chi^\dagger i \partial^\mu \chi \right] - e^2 \chi^\dagger \chi A_\mu A^\mu$$

Electromagnetic current of a charged scalar field $J^\mu = i(D^\mu \chi)^\dagger \chi - i\chi^\dagger D^\mu \chi$

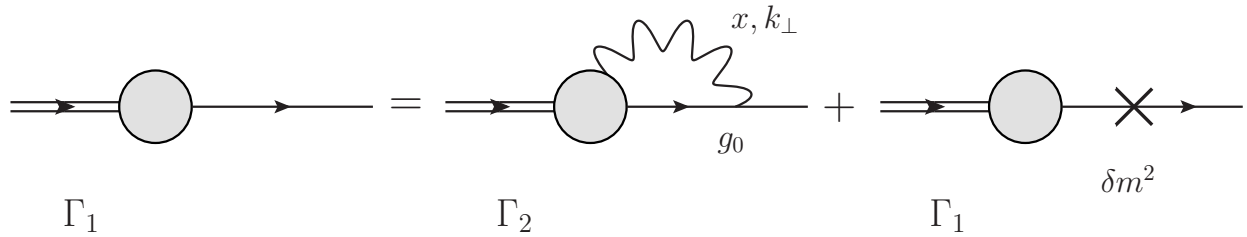
Example: electromagnetic form factor



$$
\begin{aligned}
\mathcal{M}^\mu = & \int \frac{\mathrm{d}^4 p_2}{(2\pi)^4} 2\pi\delta(p_2^2 - m^2) \frac{\mathrm{d}^4 p_2'}{(2\pi)^4} 2\pi\delta(p'^2 - m^2) \frac{\mathrm{d}^4 p_1}{(2\pi)^4} 2\pi\delta(p_1^2 - m^2) \\
& \times \int \frac{\mathrm{d}\tau}{2\pi} \frac{1}{\tau - i\epsilon} \int \frac{\mathrm{d}\tau'}{2\pi} \frac{1}{\tau' - i\epsilon} (2\pi)^4 \delta^4(p_1 + p_2 - p - \omega\tau) \\
& \times (2\pi)^4 \delta^4(p_2 + q - p_2') (2\pi)^4 \delta^4(p_1 + p_2' - p' + \omega\tau - \omega\tau') \\
& \times \Gamma_2(p_1, p_2; p) \Gamma_2^*(p_1, p_2'; p') e (p_2 + p_2')^\mu \\
\Rightarrow \; F(q^2) = & \int \frac{\mathrm{d}^3 p_1}{(2\pi)^3 2p_1^+} \frac{\Gamma_2(p_1, p_2; p)}{s_2 - p^2} \frac{\Gamma_2^*(p_1, p_2'; p')}{s_2 - p'^2} \frac{(p_2 + p_2')^+}{(p + p')^+} \frac{p^+ p'^+}{p_2^+ p_2'^+} \\
= & \int \frac{\mathrm{d}x}{2x(1-x)} \frac{\mathrm{d}^2 k_\perp}{(2\pi)^3} \psi_2(x, k_\perp) \psi_2^*(x', k_\perp') \frac{2 - x - x'}{2(1 - x')}
\end{aligned}
$$

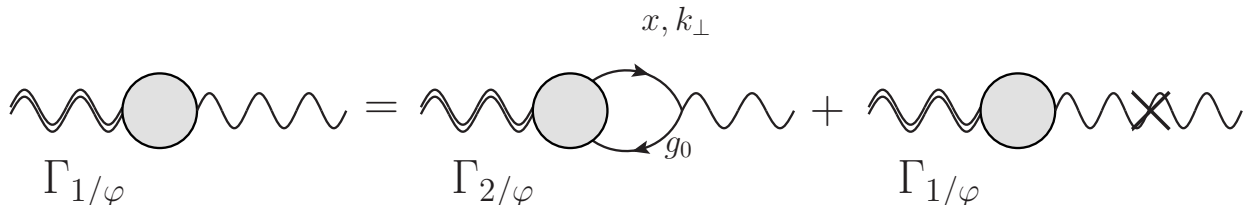
Mass renormalization

$\Gamma_1 = (s_1 - m^2)\psi_1 \to 0$, with $s_1 = p^2 = m^2 = m_{\text{ph}}^2$.



(Mass) gap equation:

$$0 = \Gamma_1 = \int \frac{\mathrm{d}x}{2x(1-x)} \frac{\mathrm{d}^2 k_\perp}{(2\pi)^3} \frac{g_0 \Gamma_2(x, k_\perp)}{s_2 - m^2} - \delta m^2 \psi_1.$$



Exercise: write down the gap equation for the φ

Field renormalization

A natural normalization in the Hamiltonian formalism is,

$$\langle \psi_\alpha(p)|\psi_\beta(p')\rangle = \delta_{\alpha\beta} 2p^+ (2\pi)^3 \delta^3(p-p').$$

In terms of the wave functions,

$$1 = |\psi_1|^2 + \int \frac{\mathrm{d}x}{2x(1-x)} \frac{\mathrm{d}^2 k_\perp}{(2\pi)^3} \left|\psi_2(x,k_\perp)\right|^2 + \cdots$$

Alternatively, we can normalize the state vector such that $\psi_1 = 1$:

$$\langle \alpha, p|\psi_\beta(p')\rangle = \delta_{\alpha\beta} 2p^+ (2\pi)^3 \delta^3(p-p').$$

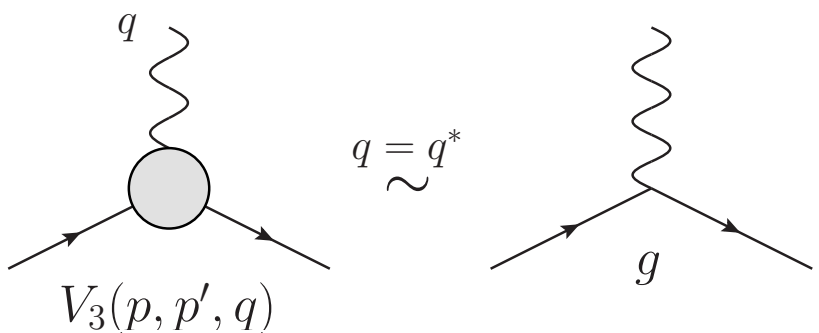
Equivalently, $\langle 0|\chi(0)|\psi(p)\rangle = 1$

Coupling constant renormalization

Tree level amplitude defines the physical coupling:

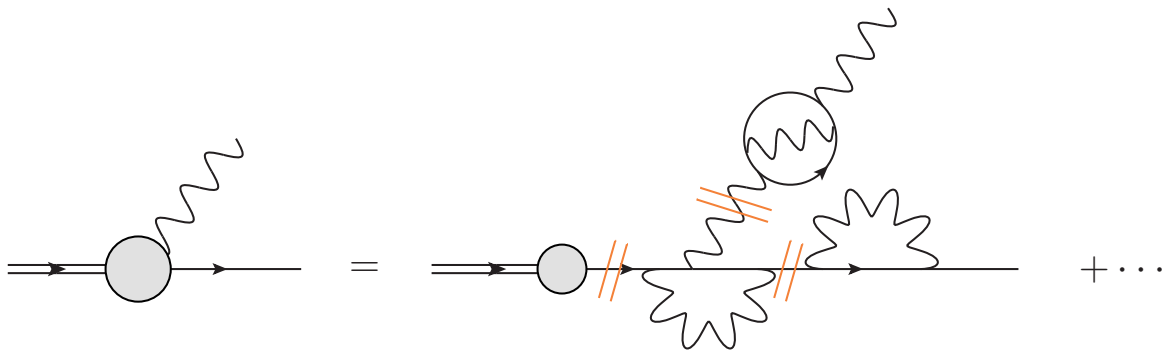
$$i\mathcal{M} = \frac{i\sqrt{Z_\chi^2 Z_\varphi}V_3(p,p',q)}{q^2-\mu^2+i\epsilon} \overset{q^2\to\mu^2}{\sim} \frac{ig}{q^2-\mu^2+i\epsilon}$$

where V_3 is the one-particle irreducible (1PI) vertex 3-point functions, viz. its external legs are replaced by asymptotic states, provided, the fields are renormalized.



Coupling constant renormalization

A dissection of the three-point vertex function Γ_2:



$$\Gamma_2 = \sqrt{Z_\chi} V_3 Z_\varphi^{(\text{off})} Z_\chi^{(\text{off})}$$

Therefore, the renormalization condition becomes,

$$\Gamma_2(x^*, k_\perp^*) = g\sqrt{Z_\varphi}\sqrt{Z_\chi}$$

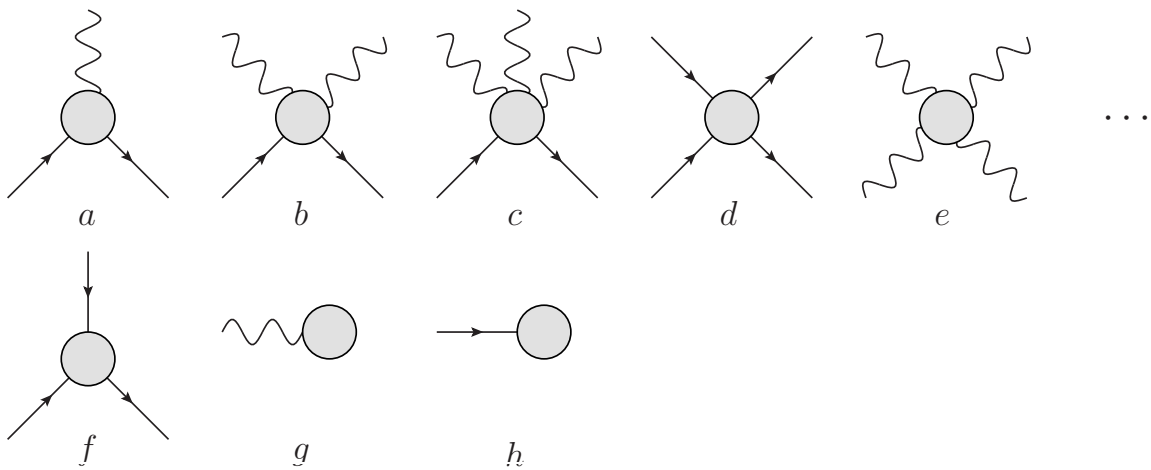
where $s_2^* = m^2$ defines the on shell condition.

Discussion on Dec. 3, 2021

Induced vertices

Are the three examples (mass, coupling, field strength) exhaustive -- in other words, are there any other quantities that need to be renormalized?

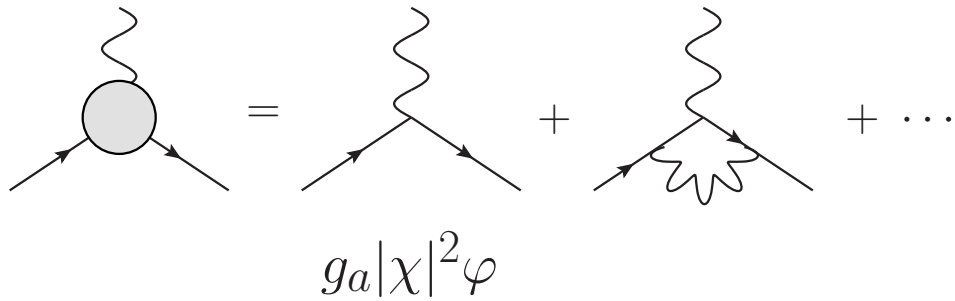
- To answer this question, let us first consider a theory with vanishing bare mass $m_0 = 0$. Are we free from the mass renormalization?
  In general, no! Because the loop still exists (unless some symmetry forbids the generation of mass, e.g. chiral symmetry for fermions).
- In the same token, we need to consider all possible induced vertices due to quantum fluctuation! (Unless a vertex is forbidden by symmetry)



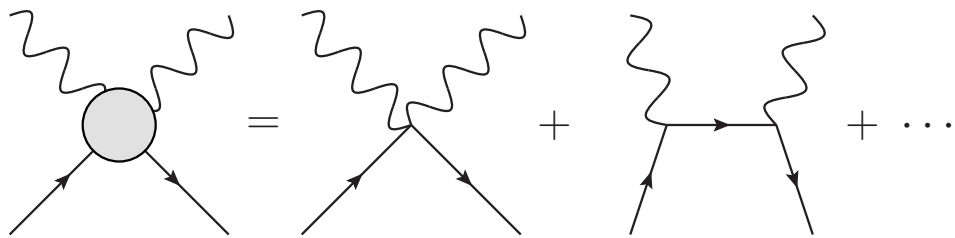
Vertices a-e are possible induced vertices, while f-h are forbidden by charge and/or Lorentz symmetries.

Induced vertices

As we mentioned, quantum fluctuations would generate all possible vertices allowed by the symmetries of the system.



$$g_a|\chi|^2\varphi$$



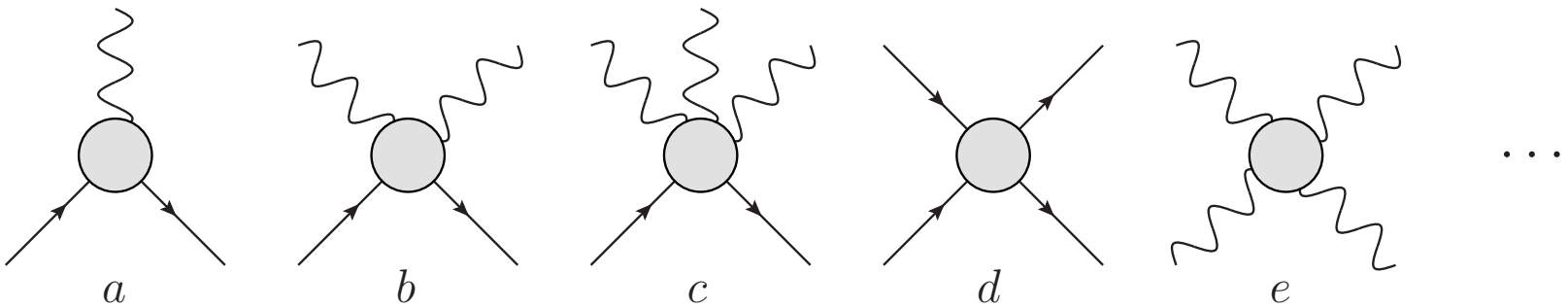
$$g_b|\chi|^2\varphi^2$$

Consider an induced $\chi\chi\varphi\varphi$ interaction. The physical coupling is determined by the induced vertex at some chosen kinematical point, and is in general non-zero.

A local operator has a bare coupling. Is this coupling zero or non-zero? Ultimately, it is determined from matching the physical coupling to the experimental measurement.

Effective field theory

Therefore, we can associate each induced vertex with a local interaction whose strength is described by a coupling constant.



$$g_a|\chi|^2\varphi \qquad g_b|\chi|^2\varphi^2 \qquad g_c|\chi|^2\varphi^3 \qquad g_d|\chi|^4 \qquad g_e\varphi^4$$

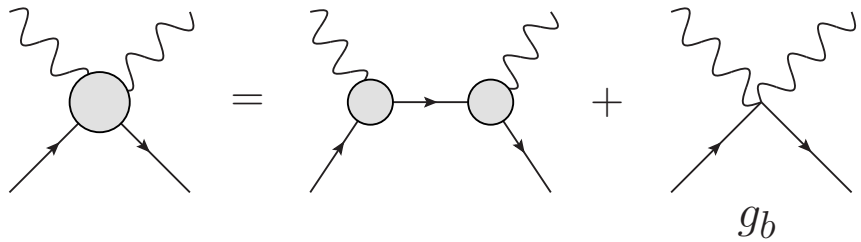
Each set of (physical) couplings define a theory (including the masses). At this point, the couplings have to be determined from measurement of physical observables.

$$\mathscr{L} = -\chi^\dagger\left[\partial^2 + m^2\right]\chi - \tfrac{1}{2}\varphi\left[\partial^2 + \mu^2\right]\varphi + \sum_i g_i O_i(|\chi|^2, \varphi)$$

Effective NN interactions

Example: using Yukawa theory to describe the nuclear force.

- Assume pion and nucleon are separately studied and their masses μ, m are known. Assume the π-N coupling g_a is known e.g. from experiments.
- Now, consider the $\pi\pi N$ scattering experiment. The result is likely different from the π-N coupling theory prediction. This determines g_b.



- Similar multi-πN scattering experiments determine the π-N couplings $g_{a,b,c,\ldots}$. The N-N scattering experiments determines the NN couplings $g_{d,\ldots}$.
- In order to make the process tractable, we work with a low pion energy $Q \ll \Lambda$ where the nucleon-anti-nucleon fluctuation can be ignored.
- For an A-nucleon system, there may be up to A-body interactions. QFT in principles allows a fluctuation up to an infinite number of particles.
- Predictive power lies within the access to other observables

Wait a second!

- This is not what I learned from QFT classes!
  What we learned from QFT classes are based on leading-order perturbation theory. And we are satisfied with that due to the complication in algebra. Many things (including deeper questions) are ``forbidden'' by the lack of know-how.

- How could this be useful?
  It is so ironic that in fundamental science we do not know the fundamental quantum theory, the quantum Hamiltonian. In applied sciences, the details of the quantum theory, like the properties of the electrons are given.

- Are there something missing?
  Yes, to make the theory useful. It is separation of scales.

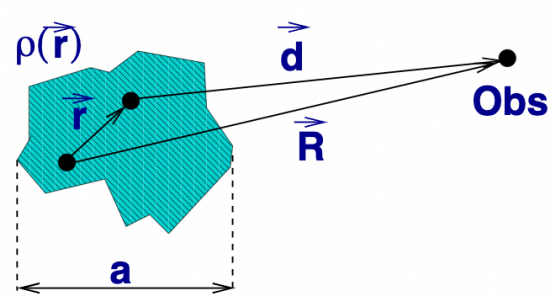
Multipole expansion as an effective theory

Consider the electric potential $\varphi(\vec{r})$ generated by a charge distribution ρ:

$$\varphi(\vec{R}) = \int \mathrm{d}^3 r \frac{\rho(\vec{r})}{|\vec{r} - \vec{R}|}$$

$$= \sum_{n=0}^{\infty} \frac{1}{R^{n+1}} \underbrace{\int \mathrm{d}^3 r \rho(\vec{r}) r^n P_n(\cos\theta)}_{q_n, \text{ multipole moments}}$$

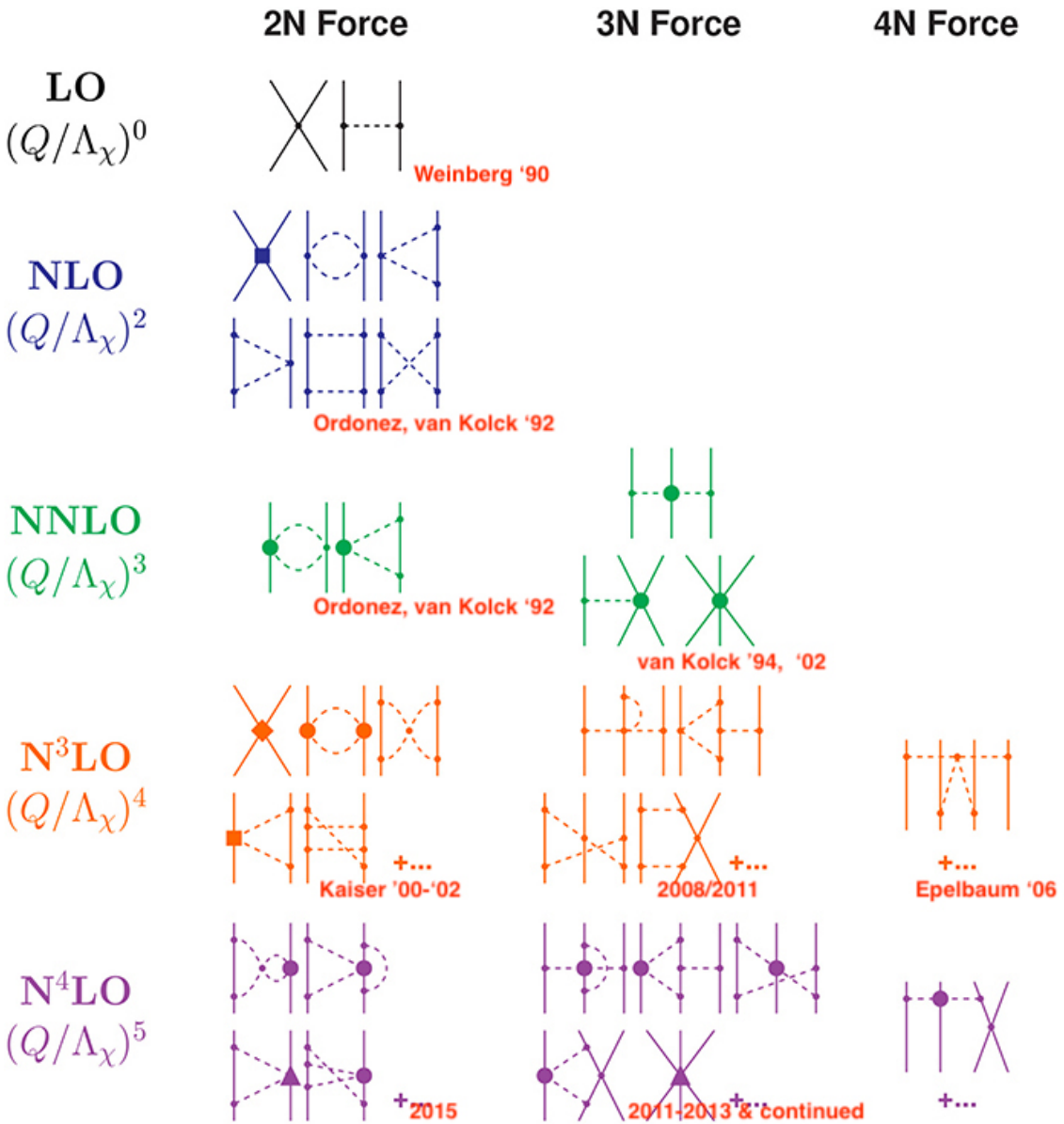
$$= \sum_{n=0}^{\infty} \frac{q_n}{R^{n+1}} = \frac{q}{R} + \frac{p}{R^2} + \frac{Q}{R^3} + \cdots$$



In this example,

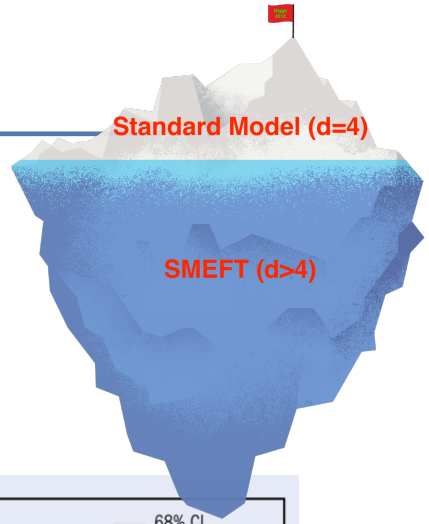
- We need an infinite number of couplings -- multipole moments
- Only valid & useful with the separation of scales $a \ll R$
- High moments are suppressed by the power of a/R if the multipole moments are ``natural''
  - *Naturalness:* $q_n \equiv a^n \bar{q}_n$, *where the dimensionless moment* $\bar{q}_n \sim O(1)$
  - *There could be exact symmetries that eliminate* $\bar{q}_n$ *completely. For example, composite particles with spin* J *only has up to* $2J+1$ *multipoles (electric + magnetic).*
  - *A super large* $\bar{q}_n \gg 1$ *or a super-tiny* $\bar{q}_n \ll 1$ *(but* $\bar{q}_n \neq 0$*) are all unnatural cases.*

Chiral effective field theory

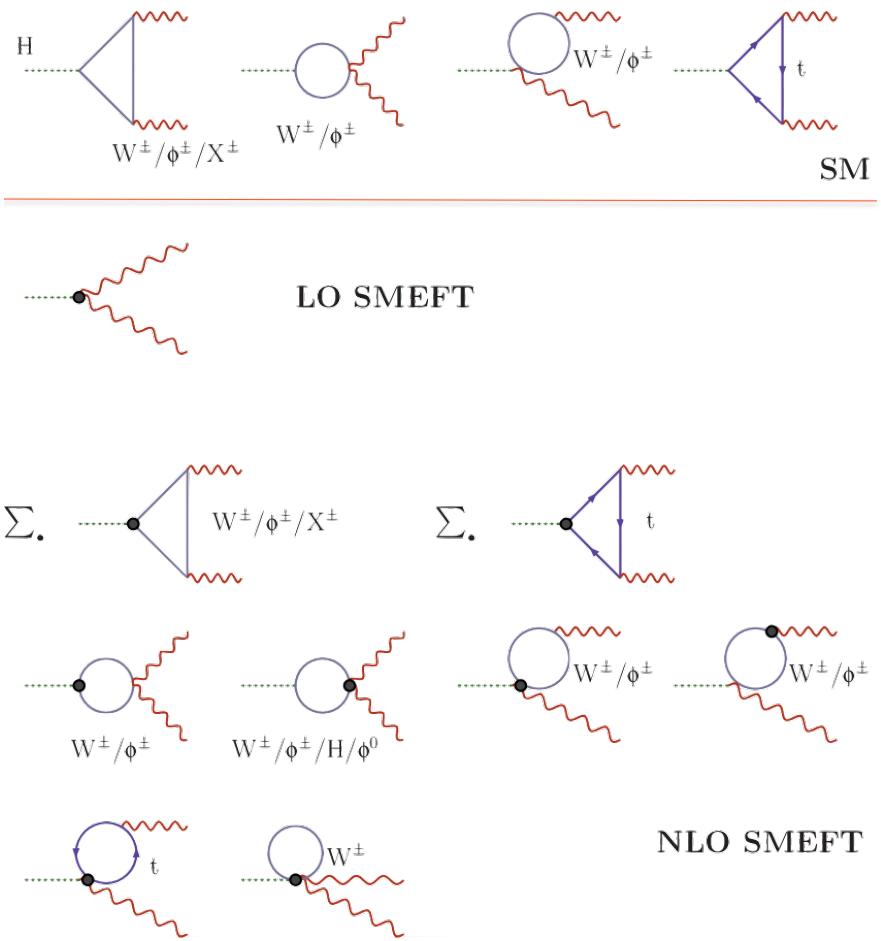


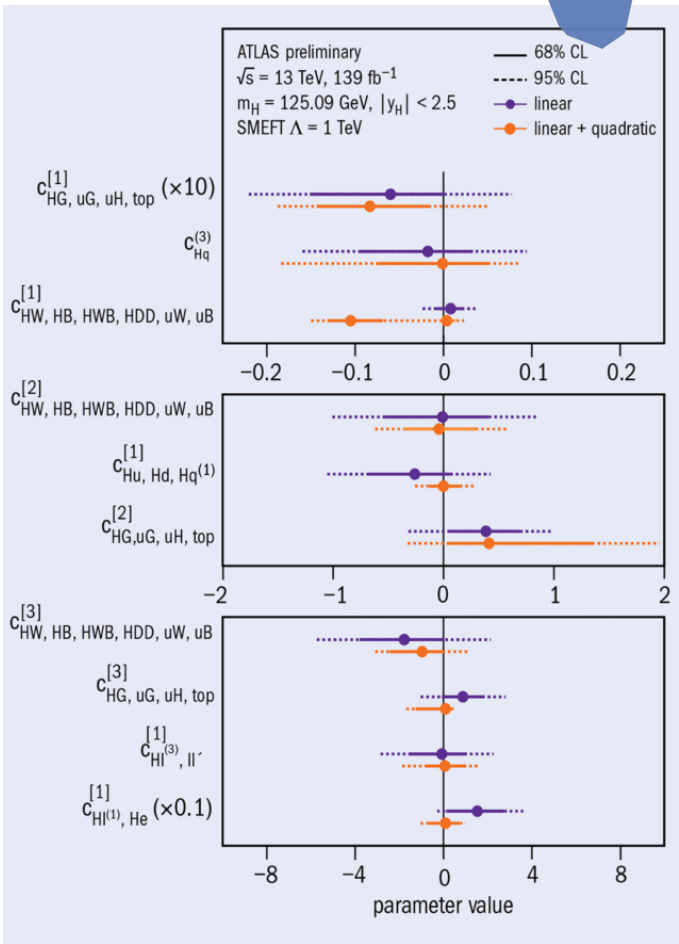
Modern nuclear force from χEFT

Standard Model as an EFT

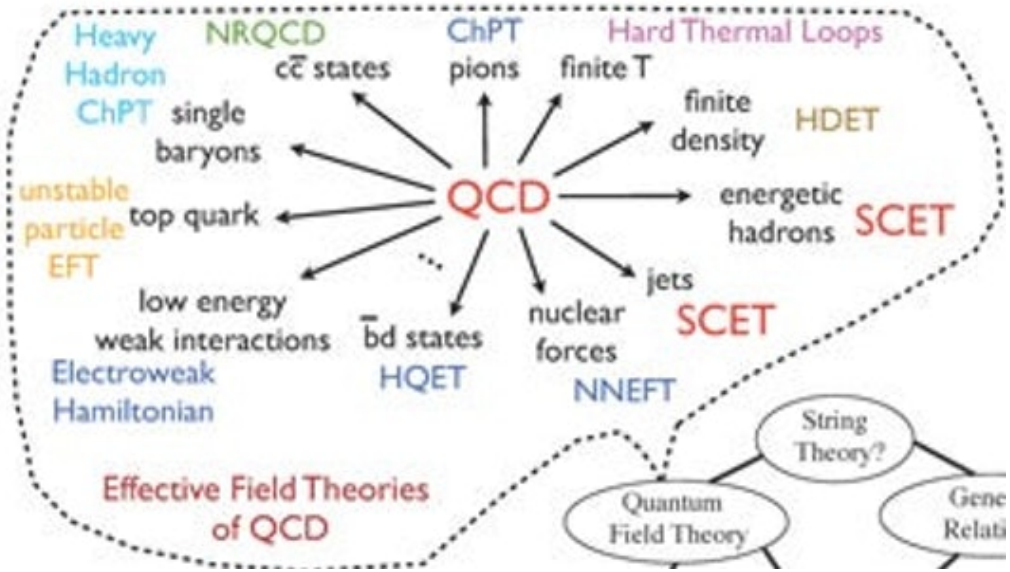


$$\mathscr{L}_{\text{SMEFT}} = \mathscr{L}_{\text{SM}} + \sum_{i=1}^{2499} \frac{C_i^{(6)}}{\Lambda^2} O_i^{(6)} + \sum_i \frac{C_i^{(8)}}{\Lambda^4} O_i^{(8)} + \cdots$$





All Things EFT



MOOCs:

- MIT OpenCourseWare: Effective Field Theory (Spring 2013)
- All Things EFT:
  `https://sites.google.com/view/all-things-eft`

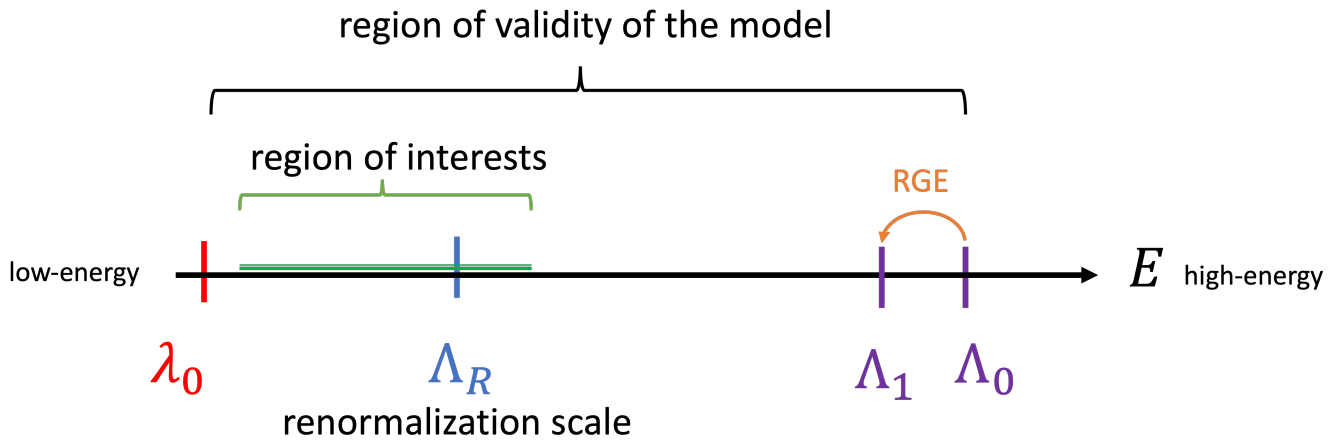
Separation of scales

- Local theories
  The core problem of renormalization is our lack of knowledge of the short-distance behavior.

- When the scales are well separated, details of the microscopic physics should not affect the macroscopic behaviors.
  - *Abundant examples. But, there are also counterexamples!*
  - *The microscopic physics only enters the macroscopic physics through the fundamental parameters (mass, charge, ...)*
  - *Classical theories are naturally compatible with the principle of separation of scales.*
  - *Quantum fluctuations made the separation of scales in quantum fields non-trivial.*

- Low-energy constants: masses, few-body couplings.
  Ideally, the theory should be able to be described by these low-energy constants, modulo power suppressed high-energy parameters $\lambda_{low} / \Lambda_{high} \ll 1$.

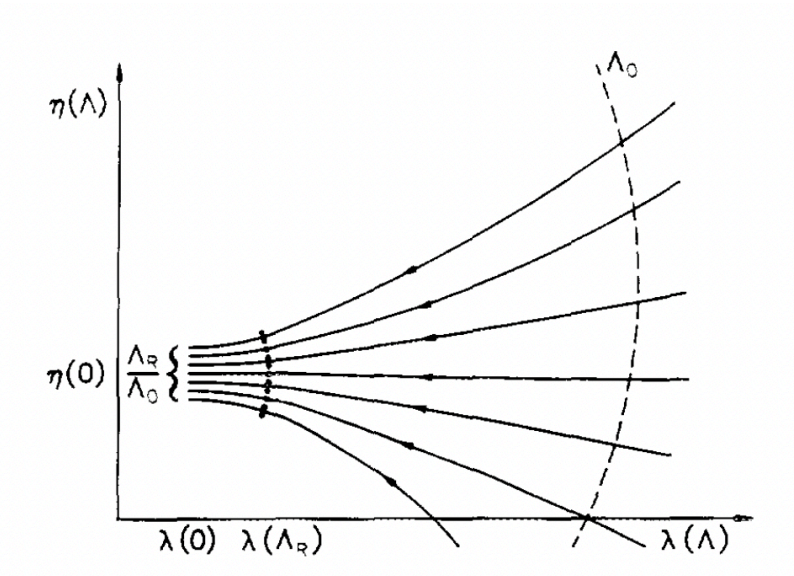
Wilsonian picture

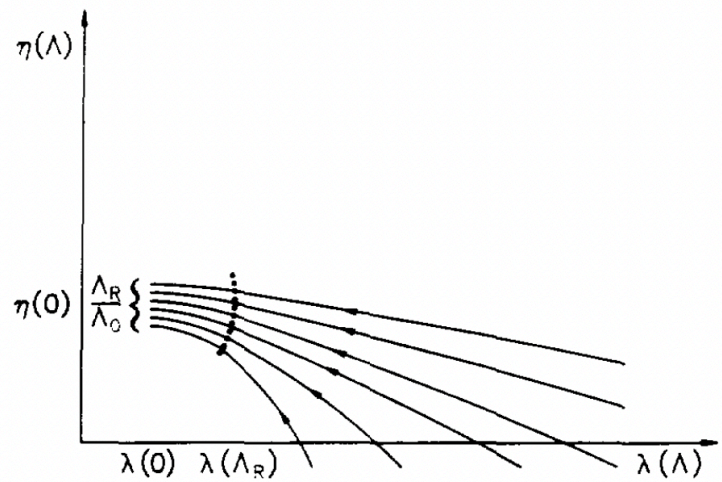


- In the Wilsonian picture, a QFT $\mathscr{L}(\{\eta_i(\Lambda_0)\}, \Lambda_0)$ $(i = 1, 2, \cdots, N)$ is defined only up to a cutoff scale $\Lambda_0 \gg \Lambda_R$ (Λ_R is the scale of interests). It contains all possible interaction terms allowed by the symmetry.
  - *The dimensionless bare parameters $\{\bar{\eta}_i\}$ should be natural.*
- The change of cutoff $\Lambda_0 \to \Lambda_1$ will make the parameters of the theory $\{\eta_i(\Lambda_1)\}$ change while keeping the physical predictions unchanged.
  - *The change of the cutoff is continuous and is called a renormalization group evolution (RGE).*
  - *In coordinate space view, RGE is the coarse-graining (smoothing) of the theory.*
  - *It comes with different versions. In general, very complicated.*

RG flow

- At the scale of interests $\Lambda_R \ll \Lambda_0$, some theories may be described by only a finite number of parameters $\{\lambda_a\}$, up to an accuracy in the power of Λ_R / Λ_0.
  - $\{\lambda_a\}$ *can be determined by experimental measurements.*
  - *Predictive power is regained.*
  - *The bare parameters* $\{\eta_i(\Lambda_R)\}$ *still exist, but they become highly correlated.*
  - *Universality: up to* $O(\Lambda_R / \Lambda_0)$*, different theories, viz. different* $\{\eta_i(\Lambda_0)\}$ *may describe the same low-energy physics.*
  - *In conventional renormalizable theories,* Λ_0 *can be taken to* ∞*, and remove the values of* η_i *except for those relevant at low energies.*





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That's all for today. Thank you.