

Matrix elements with a two-hadron final state: Lellouch-Lüscher relations

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Outline

Lecture 1: Within Quantum Mechanics, relate the spectrum and matrix elements calculated on an $L \times L \times L$ torus to scattering phases and transition amplitudes.

Lecture 2: Relativistic exclusive processes: the $K \rightarrow \pi\pi$ decay; and $e^+e^- \rightarrow \pi\pi$ and applications to $(g-2)_\mu$

Lecture 3: Probing inclusive transition rates in lattice QCD.

“Scattering of particles leaves an imprint on stationary observables; our task is to decipher that imprint.”

Why QM?

It is instructive.

An approach to particle scattering that does not work in QM will surely not work in relativistic QFT.

In two-body scattering, it has been shown that the QFT case can be reduced to a QM problem in the c.m. frame à la

$$-\frac{1}{2\mu}\Delta\psi(\mathbf{r}) + \frac{1}{2}\int d^3r' U_{\mathcal{E}}(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}') = \mathcal{E}\psi(\mathbf{r}), \quad \text{2-particle energy} = 2\sqrt{m^2 + m\mathcal{E}}$$

M. Lüscher, Commun. Math. Phys. 105, 153-188 (1986)

1d case: scattering states on the circle

[Lüscher Comm.Math.Phys. 105, 153 (1986)]

Consider a one-dimensional QM problem,

$$\begin{aligned}\psi(x, y) = f(x - y) &= f(y - x) \\ \left\{ -\frac{1}{m} \frac{d^2}{dz^2} + V(|z|) \right\} f(z) &= E f(z).\end{aligned}$$

Scattering state: for $E = k^2/m$, $k \geq 0$, choose

$$f_E(z) \stackrel{|z| \rightarrow \infty}{\sim} (1 + \dots) \cos(k|z| + \delta(k))$$

- now consider a finite periodic box, $L \gg$ range of V
- $V_L(z) = \sum_{\nu \in \mathbb{Z}} V(|z + \nu L|)$
- in leading approx., $f_E(z)$ unchanged, but quantization condition:

$$f'_E(-\frac{L}{2}) = f'_E(\frac{L}{2}) = 0 \quad \Rightarrow \quad \boxed{\frac{1}{2}kL + \delta(k) = \pi n, \quad n \in \mathbb{Z}.}$$

Generalization to 3d?

Lüscher's condition: quantum mechanics analysis (I)

M. Lüscher B354 (1991) 531

Two spinless particles in the final state, interacting via a short-range potential of range R ; reduced mass $\mu = (1/m_1 + 1/m_2)^{-1}$.

A. Scattering state in infinite volume in the rest frame:
wavefunction $\psi(\mathbf{x}_1 - \mathbf{x}_2)$

For $r >$ interaction range, ψ satisfies the free stationary Schrödinger equation (i.e. the Helmholtz equation)

$$(\Delta + k^2)\Psi(\mathbf{r}) = 0, \quad E = \frac{k^2}{2\mu}.$$

Solution via spherical Bessel functions,

$$\psi(\mathbf{r}) = Y_{\ell m}(\theta, \phi) \left(\alpha_{\ell}(k) j_{\ell}(kr) + \beta_{\ell}(k) n_{\ell}(kr) \right), \quad r > R.$$

Scattering phase δ_{ℓ} for final state with angular momentum ℓ :

$$e^{2i\delta_{\ell}} = \frac{\alpha_{\ell}(k) + i\beta_{\ell}(k)}{\alpha_{\ell}(k) - i\beta_{\ell}(k)}.$$

Lüscher's condition: quantum mechanics analysis (II)

B. On the $L \times L \times L$ torus, state with total momentum $\mathbf{P} = 0$: relative motion described by wave function $\Psi(\mathbf{r})$.

For $L/2 > r > R$, Ψ satisfies again the Helmholtz equation, but different boundary condition. Let

$$\Gamma = \left\{ \mathbf{p} \mid \mathbf{p} = \frac{2\pi}{L} \mathbf{n}, \mathbf{n} \in \mathbb{Z}^3 \right\}.$$

The fundamental solution, is (for k such that the denominator never vanishes)

$$G(\mathbf{r}; k^2) = \frac{1}{L^3} \sum_{\mathbf{p} \in \Gamma} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - k^2}, \text{ satisfying } -(\Delta + k^2)G(\mathbf{r}; k^2) = \delta_L^{(3)}(\mathbf{r}).$$

The state belongs to an irreducible representation of the cubic group. For instance, for the T_1 irrep containing the $\ell = 1, 3, \dots$ waves, one solution is

$$\Psi(\mathbf{r}) = v_{1,0} G_{1,0}(\mathbf{r}, k^2) = \frac{1}{2L^3} \sqrt{\frac{3}{\pi}} v_{1,0} \frac{\partial}{\partial z} \sum_{\mathbf{p} \in \Gamma} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - k^2}.$$

Origin of the quantization condition

For given energy E , the angular momentum ℓ component of the wave-function is uniquely determined up to normalization, because

- the regular solution in the region $0 < r < R$ for given energy E is unique up to overall normalization;
- it determines the value and derivative of $\psi_{\ell=1}(r = R)$;
- this then uniquely determines the wave function for $r > R$ (initial-value 2nd order ODE).

Therefore, the angular momentum ℓ component of the finite-volume wave-function must be proportional to the infinite-volume wave-function of same energy E .

However, directly calculating e.g. the $\ell = 1$ component of $G_{1,0}(r, k^2)$, this is not true for fixed L and a randomly chosen E ; it is true only for discrete values of the energy \Rightarrow quantization condition.

Math. problem: partial wave decomposition of $G_{\ell,m}(r, k^2)$

Expansion in spherical harmonics is dictated by the geometry of the cube. Since we know the r dependence must be given by $n_\ell(kr)$ and $j_\ell(kr)$, sufficient to look at $r \rightarrow 0$.

Simplest case:

$$G(\mathbf{r}, k^2) \equiv \frac{1}{L^3} \sum_{\mathbf{p} \in \Gamma} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - \mathbf{k}^2} = \underbrace{\frac{k}{4\pi} n_0(kr)}_{r \rightarrow 0 : (4\pi r)^{-1}} + \frac{1}{L} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \bar{g}_{\ell m}(q) Y_{\ell m}(\theta, \phi) j_\ell(kr).$$

E.g. $\bar{g}_{00}(q)/L = \sqrt{4\pi} \lim_{r \rightarrow 0} (G(\mathbf{r}, k^2) - \frac{1}{4\pi r})$.

Use $\int dt e^{tq} K(t, \mathbf{r})$ type representation of $G(\mathbf{r}, k^2)$ with the heat kernel

$$K(t, \mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{p} \in \Gamma} e^{i\mathbf{p} \cdot \mathbf{r} - \mathbf{p}^2 t}.$$

Result:

$$\bar{g}_{\ell m}(q) = \frac{i^\ell}{\pi q^\ell} \mathcal{Z}_{\ell m}(1; q^2), \quad q = \frac{kL}{2\pi}.$$

“3d zeta fctn”: $\mathcal{Z}_{\ell m}(s; q^2) = \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{\mathcal{Y}_{\ell m}(\mathbf{n})}{(n^2 - q^2)^s}, \quad \mathcal{Y}_{\ell m}(\mathbf{r}) \equiv r^\ell Y_{\ell m}(\theta, \phi).$

Math. problem: PW decomposition of $G_{\ell,m}(r, k^2)$ (II)

Example in the T_1 irrep:

$$G_{1,m}(\mathbf{r}) = -\frac{k^2}{4\pi} Y_{1m}(\theta, \phi) [n_1(kr) + \mathcal{M}_{1m,1m}(q) j_1(kr)] + \text{other partial waves.}$$

$\mathcal{M}_{\ell m, \ell' m'}(q)$ = combination of 3d zeta functions and Clebsch-Gordan coefficients.

Compare the expression with infinite-volume wave function

$$\psi_{1,m}(\mathbf{r}) \stackrel{r \geq R}{=} Y_{1,m}(\theta, \phi) \left(\alpha_1(k) j_1(kr) + \beta_1(k) n_1(kr) \right)$$

\Rightarrow quantization condition:

$$\alpha_1(k) - \beta_1(k) \mathcal{M}_{1m,1m}(q) = 0.$$

More generally: $\det[A - BM] = 0$.

The main practical result for the spectrum

Lüscher's condition determining the spectrum in the A_1 or in the T_1 representation, neglecting all but the lowest- ℓ scattering phase (s and p wave respectively):

$$\delta_\ell(k) + \phi(q) = n\pi, \quad n \in \mathbb{Z}, \quad q \equiv \frac{kL}{2\pi}.$$

$\phi(q)$ a known, continuous kinematic function; $\phi(0) = 0$ and

$$\tan \phi(q) = -\frac{\pi^{3/2}q}{\mathcal{Z}(1; q^2)}, \quad \mathcal{Z}(s; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{n \in \mathbb{Z}^3} \frac{1}{(n^2 - q^2)^s}.$$

Non-relativistic quantum mechanics: $E = \frac{k^2}{2\mu}$.

Not obvious, but in a relativistic theory, the only change is that $E = 2\sqrt{k^2 + m^2}$.

Analytically continuing zeta functions

For $\text{Re}(s) > 1$:

$$\zeta(s) \equiv \sum_{n \geq 1} \frac{1}{n^s} = \sum_{n \geq 1} \frac{1}{\Gamma(s)} \int_0^\infty dt t^{s-1} e^{-tn} = \frac{1}{\Gamma(s)} \int_0^\infty dt \frac{t^{s-1}}{e^t - 1}.$$

Now

$$\zeta(s) = \frac{1}{\Gamma(s)} \left\{ \int_0^1 dt t^{s-2} + \int_0^1 dt t^{s-1} \left[\frac{1}{e^t - 1} - \frac{1}{t} \right] + \int_1^\infty dt \frac{t^{s-1}}{e^t - 1} \right\}.$$

The analytic continuation to $\text{Re}(s) > 0$ can now be performed by replacing $\int_0^1 dt t^{s-2}$ by $\frac{1}{s-1}$.

$$\sum_{n \in \mathbb{Z}} \frac{1}{(n^2 - q^2)^s} = \sum_{|n| < \lambda} \frac{1}{(n^2 - q^2)^s} + \frac{1}{\Gamma(s)} \int_0^\infty dt t^{s-1} e^{tq^2} \sum_{|n| \geq \lambda} e^{-tn^2}$$

for $\lambda^2 > \text{Re}(q^2)$. Then proceed in the same way to continue to the region $\text{Re}(s) \leq \frac{1}{2}$.

The case of the 3d $\mathcal{Z}_{\ell m}(s; q^2)$ is analogous.

Normalization of the states (I)

∞ Vol: $\psi(\mathbf{r}) = Y_{\ell m}(\theta, \phi) (\alpha_{\ell}(k)j_{\ell}(kr) + \beta_{\ell}(k)n_{\ell}(kr))$, $r >$ interaction range

Torus: $\Psi(\mathbf{r}) = v_{1,0} G_{1,0}(\mathbf{r}, k^2) = \frac{1}{2L^3} \sqrt{\frac{3}{\pi}} v_{1,0} \frac{\partial}{\partial z} \sum_{\mathbf{p}} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\mathbf{p}^2 - k^2}$.

◆ Lüscher's condition determining the spectrum:

$$\delta_{\ell}(k) + \phi(q) = n\pi, \quad n \in \mathbb{Z}, \quad q \equiv \frac{kL}{2\pi}.$$

◆ What value of $v_{1,0}$ normalizes the wavefunction to unity? Use a trick:

[Lellouch, Lüscher hep-lat/003023; HM 1202.6675]

$$\delta_{\ell} \quad \xrightarrow{(L)} \quad E_n(L)$$

$$\downarrow \Delta V \quad \quad \quad \downarrow \Delta V$$

$$\delta_{\ell} + \Delta\delta_{\ell} \quad \xrightarrow{(L)} \quad E_n(L) + \Delta E_n(L).$$

Normalization of the states (II)

1st order perturbation theory in quantum mechanics under $V \rightarrow V + \Delta V$:

$$\Delta E = \int_{\Omega_L} d^3\mathbf{r} \Psi(\mathbf{r})^* \underbrace{Q_\Lambda}_{\text{projector onto } \ell \leq \Lambda} \Delta V_L(\mathbf{r}) \Psi(\mathbf{r}) = \frac{dE}{dk} \Delta k.$$

On the other hand, the change in the phase shift is given by the generalized Born formula (see e.g. Landau & Lifshitz, Quantum Mechanics, parag. 133), which for an energy-normalized wavefunction takes the form

$$\Delta\delta_\ell = -\pi \int_0^\infty r^2 dr \Delta V(r) |\psi_{\ell m}(r)|^2.$$

Taking the differential of the quantization condition, the change in the scattering phase is accompanied by a change in the energy level according to

$$\Delta\delta_\ell(k) = -F_\ell(k, L) \frac{\Delta k}{k}, \quad F_\ell(k, L) \equiv k \frac{\partial\delta_\ell(k)}{\partial k} + q\phi'(q).$$

$F_\ell(k, L)$ is the Lellouch-Lüscher factor.

Putting these three equations together, we obtain...

Relation between finite- and infinite volume wavefunction

$$|\psi_{1,m}(r)|^2 = \frac{dk}{dE} \cdot \frac{F_1(k, L)}{\pi k} \cdot |\Psi_{1,m}(r)|^2, \quad (r < L/2).$$

- infinite volume normalization of states:

$$\psi(\mathbf{r}; E) = Y_{1m}(\theta, \phi)\psi_{1m}(r; E), \quad \int d^3r \psi(\mathbf{r}; E)\psi(\mathbf{r}; E') = \delta(E - E');$$

- finite volume normalization of states:

$$\Psi(\mathbf{r}) = \sum_{\ell, m} Y_{\ell m}(\Omega)\Psi_{\ell m}(r), \quad \int_0^L d^3\mathbf{r} |\Psi(\mathbf{r})|^2 = 1.$$

$$F_\ell(k, L) \equiv k \frac{\partial \delta_\ell(k)}{\partial k} + q\phi'(q), \quad E(k) = \frac{k^2}{2\mu}.$$

Higher partial-wave content of the finite-volume state

Writing

$$\Psi(\mathbf{r}) = v_{1\bar{m}} G_{1m}(\mathbf{r}, k^2) = v_{1\bar{m}} \sum_{\ell=1,3,\dots} Y_{\ell\bar{m}}(\theta, \phi) \Psi_{\ell\bar{m}}(\mathbf{r}),$$

the relation on the previous slide shows that

$$v_{1\bar{m}} = -\sqrt{\frac{2\mu}{F_1(k, L)} \frac{dE}{dk}} \frac{4\pi}{k} \sin \delta_1.$$

For $\ell = 3, 5, \dots$,

$$\Psi_{\ell\bar{m}}(\mathbf{r}) = -\frac{k^2}{4\pi} v_{1\bar{m}} \mathcal{M}_{1\bar{m}, \ell m}(q) j_\ell(kr).$$

Coupling the particles to photons [HM, 1202.6675]

Couple the two (interacting) particles to electromagnetic radiation. With

$$\mathbf{R} = \frac{m_a \mathbf{r}_a + m_b \mathbf{r}_b}{M}, \quad \mathbf{r} = \mathbf{r}_b - \mathbf{r}_a \quad (M = m_a + m_b),$$

the matter-radiation Hamiltonian can be written in the form

$$H_{\text{kin}} = \frac{1}{2M} (\mathbf{P} - (e_a \mathbf{A}_a + e_b \mathbf{A}_b))^2 + \frac{1}{2\mu} \left(\mathbf{p} - \mu \left(\frac{e_b}{m_b} \mathbf{A}_b - \frac{e_a}{m_a} \mathbf{A}_a \right) \right)^2$$

- $\mu = \frac{m_a m_b}{m_a + m_b}$ = reduced mass of the two particles
- $\mathbf{A}_c \equiv \mathbf{A}(\mathbf{r}_c)$
- e_c is the electric charge ($c = a, b$)
- the non-vanishing commutation relations are $[P_i, R_j] = [p_i, r_j] = -i\delta_{ij}$.

Applying Fermi's golden rule

Transition rate: $\frac{dP}{dt} = 2\pi |\langle \Psi_f | h_I | \Psi_i \rangle|^2 \rho(E_f)$,
where $\rho(E) = \frac{dn}{dE}$ is the density of final states.

FGR assumes Ψ_f and Ψ_i are unit-normalized. If instead $|\Psi_f\rangle$ is energy-normalized, meaning

$$\langle \Psi_f(E) | \Psi_f(E') \rangle = \delta(E - E'),$$

then $\rho(E_f)$ can be set to unity.

The transition is forbidden unless spatial momentum is conserved:
if $|\psi_{f,i}\rangle = L^{3/2} |\Psi_{i,f}\rangle$, can write

$$\langle \psi_f | h_I | \psi_i \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{P} - \mathbf{P}') \cdot A, \quad A = \langle \Psi_f | h_I | \Psi_i \rangle.$$

From then on, work with the $|\psi_{f,i}\rangle$.

In quantum mechanics, $\langle \mathbf{R} \mathbf{r} | \psi_f \rangle = e^{i\mathbf{P}' \cdot \mathbf{R}} \psi_{f,\ell}(r) Y_{\ell m}(\theta, \phi)$ with
 $\int_0^\infty dr r^2 \psi_{f,\ell,E}(r) \psi_{f,\ell,E'}^*(r) = \delta(E - E')$.

Transition in infinite volume (I)

One-photon transitions driven by the term

$$h_I = -\frac{1}{2} \left\{ \mathbf{p}, \left(\frac{e_b}{m_b} \mathbf{A}_b - \frac{e_a}{m_a} \mathbf{A}_a \right) \right\}$$

(and a second term $H_I = -\frac{1}{2M} \{ \mathbf{P}, e_a \mathbf{A}_a + e_b \mathbf{A}_b \}$, but the latter is subdominant at long wavelengths).

Consider a transition from an s-wave bound state ψ_i to a final state ψ_f with angular momentum eigenvalues ($\ell = 1, m = \sigma$). Using Fermi's Golden Rule, transition rate given by $\frac{dP}{dt} = 2\pi |\langle \psi_f | h_I | \psi_i \rangle|^2 \rho(E_f)$; divide by the photon flux ($= c$) to get the cross-section.

Expand photon field in plane waves ($[a_{\mathbf{k},\sigma}, a_{\mathbf{k}',\sigma'}] = (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}') \delta_{\sigma\sigma'}$):

$$\mathbf{A}(t, \mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} \frac{\sum_{\sigma}}{\sqrt{2\omega_k}} \left(a_{\mathbf{k},\sigma} \boldsymbol{\epsilon}_{\sigma}(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + a_{\mathbf{k},\sigma}^{\dagger} \boldsymbol{\epsilon}_{\sigma}(\mathbf{k})^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \right),$$

Use $\boldsymbol{\epsilon}_{\sigma} \cdot \{ \mathbf{p}, e^{i\mathbf{k}\cdot\mathbf{r}} \} = 2\mathbf{p} \cdot \boldsymbol{\epsilon}_{\sigma} + O(k)$ and $\mathbf{p} = i\mu[H_0, \mathbf{r}]$ to write

$$h_I = \frac{1}{-2} \int \frac{d^3k}{(2\pi)^3} \frac{\sum_{\sigma}}{\sqrt{2\omega_k}} \left\{ a_{\sigma}(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{R} - \omega_k t)} \left(\frac{e_b}{m_b} - \frac{e_a}{m_a} \right) 2i\mu [H_0, \mathbf{r} \cdot \boldsymbol{\epsilon}_{\sigma}(\mathbf{k})] + \text{h.c.} + O(k) \right\}$$

Transition in infinite volume (II)

Transition matrix element: $\langle \mathbf{R} \mathbf{r} | \psi_i \rangle = e^{-i\mathbf{k} \cdot \mathbf{R}} \psi_i(\mathbf{r})$, $\langle \mathbf{R} \mathbf{r} | \psi_f \rangle = \psi_f(\mathbf{r})$

$$A = -i\mu \frac{1}{\sqrt{2\omega}} \left(\frac{e_b}{m_b} - \frac{e_a}{m_a} \right) (E_f - E_i) \int d^3\mathbf{r} \psi_f(\mathbf{r})^* (\boldsymbol{\epsilon}_\sigma(\mathbf{k}_\gamma) \cdot \mathbf{r}) \psi_i(\mathbf{r}) + \mathcal{O}(k).$$

Kinematics of the reaction: $E_f - E_i = \omega$, $\mathbf{p}_f - \mathbf{p}_i = \mathbf{k}$.

Cross section: $\int d^3r |\psi_i(\mathbf{r})|^2 = 1$, $\int d^3r \psi_f(\mathbf{r}; E) \psi_f(\mathbf{r}; E')^* = \delta(E - E')$

$$\sigma_{\ell m}(\omega) = \delta_{\ell 1} \delta_{m\sigma} \pi \mu^2 \left(\frac{e_b}{m_b} - \frac{e_a}{m_a} \right)^2 \omega_\gamma |\boldsymbol{\epsilon}_\sigma(\mathbf{k}_\gamma) \cdot \mathbf{r}_{\text{fi}}|^2 \quad \mathbf{r}_{\text{fi}} \equiv \int d^3\mathbf{r} \psi_f(\mathbf{r})^* \mathbf{r} \psi_i(\mathbf{r}).$$

Differential cross-section:

prob. to go into p -wave \times angular prob. distribution of the p -wave $\psi_f(\mathbf{r})$

$$d\sigma = \sigma_{1\sigma}(\omega) |Y_{1,\sigma}(\theta, \phi)|^2 d\Omega \propto \sin^2(\theta) d\Omega.$$

Photodisintegration from matrix elements on the torus

- energy-levels of the final two-particle scattering state are discrete \Rightarrow tune the box size L to have all particles on-shell
- initial state has a radius $r_s < L/2 \Rightarrow$ essentially the only angular momentum component is the **s-wave component** (up to expt. corr.)
- the position operator is a pure $\ell = 1$ operator \Rightarrow
- the only partial wave that can be reached is $\ell = 1$
- the position-space contributions to $\mathbf{R}_{\text{fi}} \equiv \langle \Psi_f | \mathbf{r} | \Psi_i \rangle$ are localized at $r < r_s$
- the matrix element \mathbf{R}_{fi} would be the same as in infinite volume, if the normalization of the p -wave component of the final state were the same.

$$|\epsilon_\sigma(\mathbf{k}_\gamma) \cdot \mathbf{r}_{\text{fi}}|^2 = \frac{dk}{dE} \cdot \frac{F_1(k, L)}{\pi k} \cdot |\epsilon_\sigma(\mathbf{k}_\gamma) \cdot \mathbf{R}_{\text{fi}}|^2.$$

i.e.

$$\sigma(\omega) = 4\pi^2 \mu^2 \left(\frac{e_b}{m_b} - \frac{e_a}{m_a} \right)^2 \omega_\gamma |A|^2, \quad |A|^2 = \frac{dk}{dE} \cdot \frac{F_1(k, L)}{\pi k} \cdot \underbrace{|\langle \Psi_f | h_I | \Psi_i \rangle|^2}_{\text{on the torus, unit-norm states}}$$

Summary of lecture 1

- The quantization condition determining the finite-volume spectrum of two-particle states in terms of the infinite-volume scattering phases is derived. Main technical difficulty stems from expanding a stationary wave on the torus in spherical harmonics.
- Transitions from a bound state to a scattering state: can be computed on the torus at low energies. We saw the case of an electric dipole transition.
- Next lecture: relativistic applications.