Exact path-integral representations for the T-matrix in non-relativistic potential scattering

or:

Path Integrals for Scattering

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1. Introduction

Non-relativistic scattering of one particle in a potential $V(r)$ – in all textbooks

$\Longrightarrow$ “**uninteresting**“ ?

In the **path integral description** not totally uninteresting because

- **Path integrals** much used for the **discrete** spectrum – rarely for **scattering** (often involving infinite limits and/or formal expressions)
- New description $\Longrightarrow$ **new insights** and/or new approximations
- **Monte-Carlo methods successful for bound-state** properties (energies, masses etc.) of many-body systems or in QFT

  but **fail for scattering processes** (except for zero energy) because they can be only performed in imaginary (euclidean) time.

  New description $\Longrightarrow$ **new chance ?**

2. How to obtain a path integral representation for the T-matrix

Start with definition of S-matrix

$$\mathcal{S}_{i\to f} = \lim_{T\to\infty} \left\langle \mathbf{k}_f \,\middle|\, \hat{U}_I(T,-T) \,\middle|\, \mathbf{k}_i \right\rangle \qquad \text{(time-evolution operator in the interaction picture)}$$

$$= \lim_{T\to\infty} e^{i(E_i+E_f)T} \left\langle \mathbf{k}_f \,\middle|\, \hat{U}(T,-T) \,\middle|\, \mathbf{k}_i \right\rangle \qquad \text{(full time-evolution operator)}$$

$$=: (2\pi)^3 \delta^{(3)}\left(\mathbf{k}_i - \mathbf{k}_f\right) - 2\pi i \delta\left(E_i - E_f\right) \mathcal{T}_{i\to f} \qquad \text{(connection between } S\text{- and } T\text{-matrix)}$$

and use standard path-integral representation for matrix element of $\hat{U}(t_b, t_a)$

$$U\left(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a\right) \equiv \left\langle \mathbf{x}_b \right| e^{-i\hat{H}(t_b-t_a)} \left| \mathbf{x}_a \right\rangle = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}^3 x(t) \, \exp\left\{ i \int_{t_a}^{t_b} dt \left[\frac{m}{2}\dot{\mathbf{x}}^2(t) - V(\mathbf{x}(t)) \right] \right\}$$

Convert to **velocity path-integral** by inserting $1 = \int \mathcal{D}^3 v(t)\, \delta\left[\dot{\mathbf{x}}(t) - \mathbf{v}(t)\right]$ into the (discretized) path integral and performing the $\mathbf{x}$-functional integral.

Advantage: velocities unconstrained but boundary conditions included!

After shift of variables one then obtains

$$(\mathcal{S}-1)_{i\to f} = \lim_{T\to\infty} e^{i\Phi(T)} \int d^3r \, e^{-i\mathbf{q}\cdot\mathbf{r}} \int \mathcal{D}^3v \, \exp\left[i \int_{-T}^{+T} dt \, \frac{m}{2} \mathbf{v}^2(t) \right] \cdot \left\{ \exp\left[-i \int_{-T}^{+T} dt \, V\left(\mathbf{r} + \frac{\mathbf{K}}{m} t + \mathbf{x}_v(t) \right) \right] - 1 \right\}$$

with

$$\boxed{\mathbf{x}_v(t) := \frac{1}{2} \int_{-T}^{+T} dt' \, \mathrm{sgn}(t-t') \, \mathbf{v}(t')} \quad , \ \dot{\mathbf{x}}_v(t) = \mathbf{v}(t)$$

$$\int \mathcal{D}^3v \, \exp\left[i \int_{-T}^{+T} m\mathbf{v}^2(t)/2 \right] = 1 \qquad \text{(normalization)}$$

$\mathbf{K} = \frac{1}{2}(\mathbf{k}_i + \mathbf{k}_f)$ **mean momentum** , $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ **momentum transfer**

Two problems remain:

i) Phase $\Phi(T) = (E_i + E_f - \frac{\mathbf{K}^2}{m})\, T = \frac{\mathbf{q}^2}{4m} T$ diverges in the limit $T \to \infty$ **??**

ii) Energy conservation to extract the $\mathcal{T}$-matrix **??**

ad i) Each power of $\mathbf{q}^2$ can be obtained by applying $-\Delta$ on $\exp(-i\mathbf{q}\cdot\mathbf{r})$. Integration by parts and conversion to a shift operator by "undoing the square" gives

$$\exp\left(-\frac{i}{4m} T\,\Delta\right) = \int \mathcal{D}^3 w \, \exp\left[-i \int_{-T}^{+T} dt \, \frac{m}{2} \mathbf{w}^2(t) \pm \int_{-T}^{+T} dt \, f(t)\, \mathbf{w}(t) \cdot \nabla \right] , \quad \int_{-T}^{+T} dt \, f^2(t) = 2\,T$$

Note: kinetic energy of the "**anti-velocity**" $\mathbf{w}(t)$ is opposite to the usual kinetic energy in order to obtain a **real** shift $\Longrightarrow$ "**phantom**" d.o.f

(cf. Lee-Wick approach to Quantum Field Theory)

ad ii) **Faddeev-Popov trick**: insert

$$1 \;=\; \frac{|\mathbf{K}|}{m} \int_{-\infty}^{+\infty} d\tau \, \delta\left(\hat{\mathbf{K}} \cdot \left[\mathbf{r} + \frac{\mathbf{K}}{m}\tau \right] \right)$$

and shift integration variables

$$t \longrightarrow t+\tau\,, \qquad \mathbf{r} \longrightarrow \mathbf{r} - \frac{\mathbf{K}}{m}\tau$$

$\Longrightarrow$ action invariant (?) apart from

$$\int_{-T}^{+T} dt\,\ldots \longrightarrow \int_{-T-\tau}^{T-\tau} dt\,\ldots \qquad \text{(delicate infinite-time limits !)}$$

Then one obtains

$$\int d^3r\, e^{-i\mathbf{q}\cdot\mathbf{r}}\ldots \longrightarrow \frac{|\mathbf{K}|}{m}\int_{-\infty}^{+\infty} d\tau\,\exp\left(-i\mathbf{q}\cdot\frac{\mathbf{K}}{m}\tau\right)\int d^3r\,\delta\left(\hat{\mathbf{K}}\cdot\mathbf{r}\right)e^{-i\mathbf{q}\cdot\mathbf{r}}\ldots$$

$$= 2\pi\,\delta\left(\frac{\mathbf{q}\cdot\mathbf{K}}{m}\right)\int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}}\ldots$$

$\uparrow$ $\nwarrow$

impact parameter integral

$$\delta\left(\frac{\mathbf{k}_f^2}{2m} - \frac{\mathbf{k}_i^2}{2m}\right)$$

energy conservation

Thus

$$\mathcal{T}_{i\to f}^{(3-3)} = i\frac{K}{m}\int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}} \int \mathcal{D}^3v\,\mathcal{D}^3w\; \exp\left[i\int_{-\infty}^{+\infty} dt\, \frac{m}{2}\left(\mathbf{v}^2(t) - \mathbf{w}^2(t)\right)\right] \times \left\{ e^{i\chi^{(3-3)}(\mathbf{b},\mathbf{v},\mathbf{w}]} - 1 \right\}$$

with

$$\chi^{(3-3)}(\mathbf{b},\mathbf{v},\mathbf{w}] = -\int_{-\infty}^{+\infty} dt\, V\left(\boldsymbol{\xi}(t)\right)$$

$$\boldsymbol{\xi}(t) = \mathbf{b} + \frac{\mathbf{K}}{m}t + \mathbf{x}_v(t) - \mathbf{x}_w(0)\,, \quad \dot{\boldsymbol{\xi}}(t) = \frac{\mathbf{K}}{m} + \mathbf{v}(t)$$

$$|\mathbf{K}| = k\cos(\theta/2)\,, \quad |\mathbf{q}| = 2k\sin(\theta/2) \quad (\theta = \text{scattering angle})$$

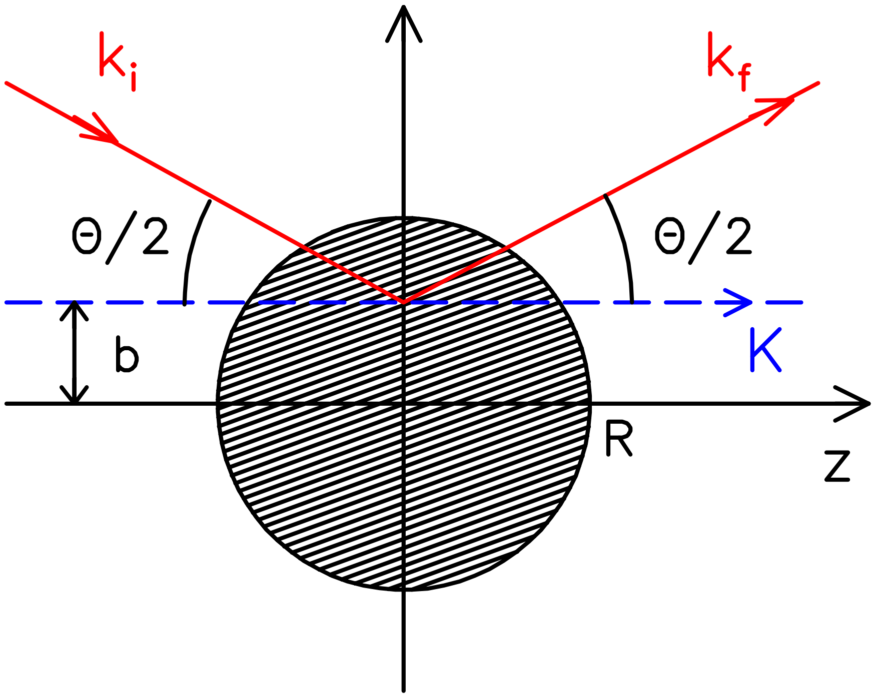
Can achieve the same with an **1-dimensional** anti-velocity by simultaneous change of velocity variables and impact parameter $\mathbf{b}$

$$\mathcal{T}_{i\to f}^{(3-1)} = i\frac{K}{m}\int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}} \int \mathcal{D}^3 v\, \mathcal{D}w\; \exp\left[i\int_{-\infty}^{+\infty} dt\, \frac{m}{2}\left(\mathbf{v}^2(t) - w^2(t)\right)\right] \times \left\{ e^{i\chi^{(3-1)}(\mathbf{b},\mathbf{q},\mathbf{v},w]} - 1 \right\}$$

with
$$\chi^{(3-1)}(\mathbf{b},\mathbf{q},\mathbf{v},w] = -\int_{-\infty}^{+\infty} dt\, V\left(\boldsymbol{\xi}_{\text{ray}}(t)\right)$$

$$\boldsymbol{\xi}_{\text{ray}}(t) = \mathbf{b} + \frac{\mathbf{p}_{\text{ray}}(t)}{m}t + \mathbf{x}_v(t) - \mathbf{x}_{v\,\perp}(0) - x_w(0)$$

$$\mathbf{p}_{\text{ray}}(t) = \mathbf{K} + \frac{\mathbf{q}}{2}\text{sgn}(t) = \mathbf{k}_i\,\Theta(-t) + \mathbf{k}_f\,\Theta(t)$$



Checked that both representations lead to the complete Born series in all orders !

3. Applications

A) High -energy expansions

At high energy and small scattering angle the particle mainly travels along a **straight-line path**. Indeed:

Expand in powers of $\mathbf{v}, \mathbf{w} \Longrightarrow$ a **systematic expansion** in powers of $1/K = 1/(k \cos(\theta/2))$ is obtained and meaningful if potential is smooth enough.

leading term:

$$\chi_{AI}^{(0)}(\mathbf{b}) = -\frac{m}{K} \int_{-\infty}^{+\infty} dz \, V\left(\mathbf{b} + \hat{\mathbf{K}} z\right)$$

eikonal approximation

Abarbanel & Itzykson (1969)

and **eikonal corrections** Wallace (1973)

Similarly one obtains a systematic $1/k$-expansion by expanding $\chi^{(3-1)}$ in powers of $\mathbf{v}$ and w (**ray-expansion**)

B) Variational approximations

Use Feynman-Jensen variational principle

$$\left\langle e^{-\Delta S} \right\rangle \geq e^{-\langle \Delta S \rangle} \; , \quad \Delta S = S - S_t$$

for complex weights $\Longrightarrow$ only **stationarity** possible

Simplest trial action motivated by eikonal expansion

$$S_t = \int dt \, \frac{m}{2} \left(\mathbf{v}^2 - w^2 \right) + \int dt \left[\underset{\uparrow}{\mathbf{B(t)}} \cdot \mathbf{v} + \underset{\uparrow}{\mathbf{C(t)}} \cdot w \right]$$

variational functions

see J. Carron, arXiv:0903.0263, Master Thesis (ETH Zurich):

impressive agreement also at higher scattering angles

C) Monte-Carlo evaluation of high-energy scattering ?

Main idea:

Damp oscillations in path integral by giving the particle a complex mass

$$\boxed{m \longrightarrow m\,(1 + i\,\mathbf{\Gamma}\,)}$$

and the phantom the complex conjugate mass $m^\star$.

Practical implementation:

- Expand velocities in harmonic oscillator wave functions

$$\begin{pmatrix} \mathbf{v}(t) \\ \mathbf{w}(t) \end{pmatrix} = \sum_{n=0}^{\infty} \begin{pmatrix} \mathbf{v}_n \\ \mathbf{w}_n \end{pmatrix} u_n\,(t/t_0)$$

  where t_0 is a characteristic time for the scattering process

- Evaluate N modes explicitly by **Monte-Carlo integration** with Gaussian weight $\exp\left[-\mathbf{\Gamma}\,\frac{m}{2}\sum_{n=0}^{N-1}\left(\mathbf{v}_n^2 + \mathbf{w}_n^2\right)\right]$

- Treat the remaining modes (from N to ∞) by the method of **partial averaging** Doll, Coalson & Freeman (1985)
- Extrapolate the numerical results to $\mathbf{\Gamma} = 0$.

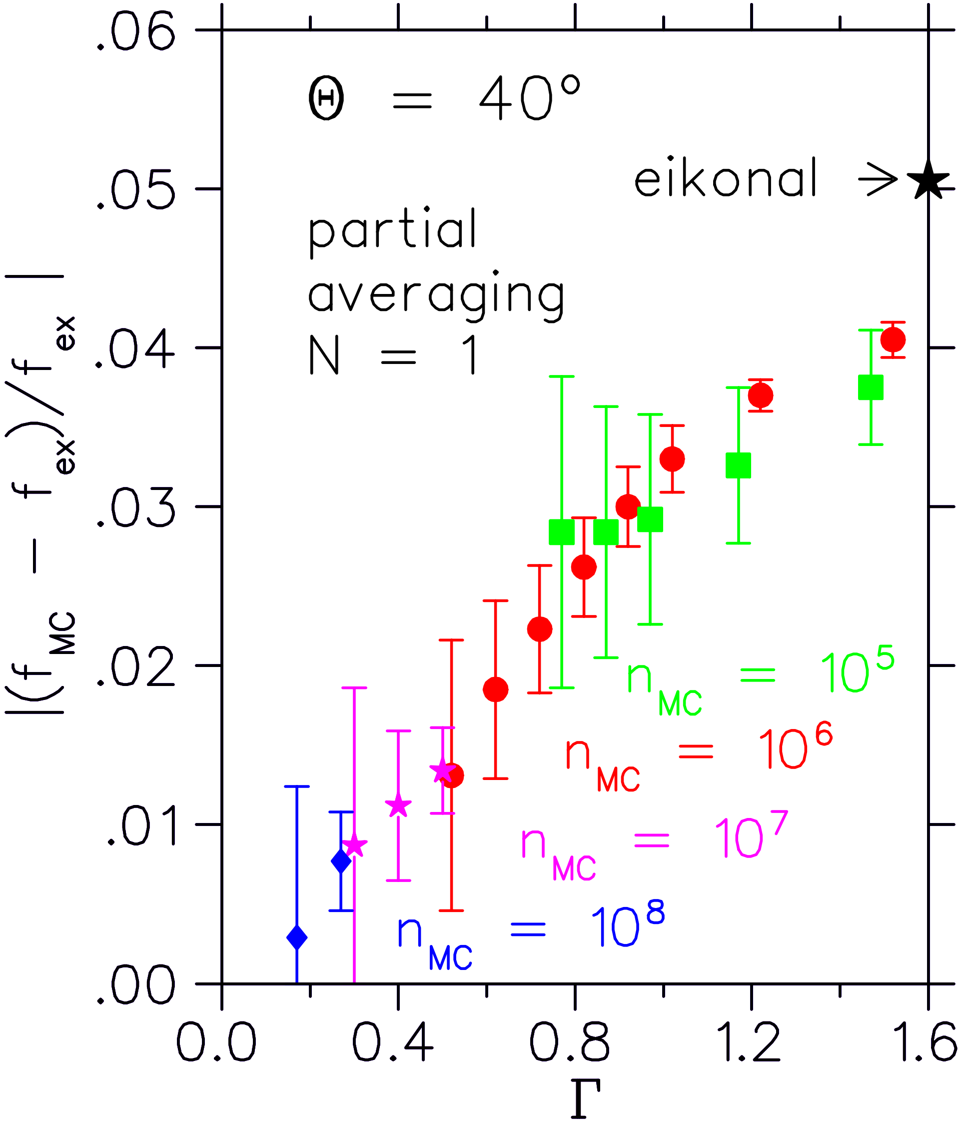
Preliminary Results:

Scattering from a **Gaussian potential**

$$V_0 \exp(-r^2/R^2) \qquad \text{with} \ \ kR = 4\,, \quad 2mV_0R^2 = -4$$

Numerical example: $\theta = 40^{o}, N = 1$. One sees that

- The numerical result at large $\mathbf{\Gamma}$ tends to the AI eikonal value.
- The smaller $\mathbf{\Gamma}$ the larger the statistical error caused by the oscillating integrand $\Longrightarrow$ the more Monte-Carlo calls are needed.
- Reasonable convergence to the exact value is obtained.


$\Theta = 40°$
eikonal →
partial
averaging
N = 1
$n_{MC} = 10^5$
$n_{MC} = 10^6$
$n_{MC} = 10^7$
$n_{MC} = 10^8$
$|(f_{MC} - f_{ex})/f_{ex}|$
.00
.01
.02
.03
.04
.05
.06
0.0
0.4
0.8
1.2
1.6
Γ

4. Possible extensions

- **Spin ?** Integrate over Grassmann-valued spin trajectory
- **Many scatterers ?** Assume $V(\mathbf{r}) = \sum_{k=1}^{N} V\left(\mathbf{r} - \mathbf{r}_k\right)$

$$\Longrightarrow \quad \exp\left(i \sum_{k=1}^{N} \chi_k \right) = \prod_{k=1}^{N} \left[1 + \left(e^{i\chi_k} - 1 \right) \right] = 1 + \sum_{j=1}^{N} \sum_{k_1 < k_2 < \ldots k_j} \prod_{l=1}^{j} \left[\exp\left(i\chi_{k_l} \right) - 1 \right]$$

multiple scattering expansion with exactly N terms!

- **Relativistic QFT ?** Assume scalar model for “nucleons” Φ (with mass M) and “mesons” χ (with mass m) and an interaction $\mathcal{L}_I = g|\Phi|^2\chi$.

With Schwinger representation for the nucleon propagator

$$\frac{1}{-\partial^2 - M^2 + g\chi + i0} = \frac{1}{2iM} \int_0^\infty dT \, \exp\left[\frac{i}{2M} \left(-\partial^2 - M^2 + g\chi \right) T \right]$$

↗

proper time

the 4-point function for scattering of two nucleons can be written in “worldline” form

$$
\begin{aligned}
G_4(x_1,x_2,x_3,x_4) \;&=\; \int_0^\infty dT_1\, dT_2 \;\text{exp}\left[-\frac{i}{2}M\,(T_1+T_2)\right] \\
&\times \int_{y_1(0)=x_1}^{y_2(T_1)=x_2} \mathcal{D}^4 y_1 \int_{y_1(0)=x_3}^{y_2(T_2)=x_4} \mathcal{D}^4 y_2 \;\text{exp}\Big(\, i\,S_0[y_1,y_2] + i\,S_{\text{int}}[y_1,y_2]\,\Big) \\
&+ \;(\, x_1 \leftrightarrow x_3\,)
\end{aligned}
$$

with

$$
S_0[y_1,y_2] \;=\; \sum_{i=1}^{2} \int_0^{T_i} d\tau \left(-\frac{M}{2}\dot{y}_i^2\right)
$$

free relativistic action

$$
S_{\text{int}}[y_1,y_2] \;=\; -\frac{g^2}{8M^2}\sum_{i,j=1}^{2}\int_0^{T_i} d\tau \int_0^{T_j} d\tau' \int \frac{d^4p}{(2\pi)^4}\,\frac{1}{\underset{\substack{\uparrow \\ \text{pion propagator}}}{p^2-m^2+i0}}\;\text{exp}\Big[-ip\cdot\big(y_i(\tau)-y_j(\tau')\big)\Big]
$$

Looks (superficially) very similar to non-relativistic description: if $i \neq j$ then 4-dimensional (retarded) analogue of scattering from a Yukawa potential !

However: **“The devil hides in the details!”** (well known since the Council of Trent)

Actually, (IMHO) there are so many “devils” that many further councils/workshops are needed in the future ...