# Path Integrals for Stochastic Scattering

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## 1. Introduction

Non-relativistic scattering of one particle in a potential $V(r)$ is covered since eons in all textbooks of Quantum Mechanics ...

$\Longrightarrow$ **topic uninteresting ?**

It depends on your point of view ...

cf. anecdote about Hardy & Ramanujan:

is the number 1729 **interesting** ?

Not totally uninteresting because

- **Path integrals** are usually employed for the **discrete** spectrum – rarely for **scattering** (and then often involving infinite limits and/or formal expressions)

- Anything different from the standard description might give you **new insights** and/or new approximations

- **Monte-Carlo methods** are **successful for bound-state** properties (energies, masses etc.) of many-body systems or in Quantum Field Theory but **fail for scattering processes** (except for zero energy) because they can be only performed in imaginary (euclidean) time. A new path integral representation might help to come closer to this long-sought goal.

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

Start with definition of $S$-matrix

$$\begin{aligned}
\mathcal{S}_{i\to f} &= \lim_{T\to\infty} \left\langle \mathbf{k}_f \,\middle|\, \widehat{U}_I(T,-T) \,\middle|\, \mathbf{k}_i \right\rangle && \text{(time-evolution operator in the interaction picture)} \\
&= \lim_{T\to\infty} e^{i(E_i+E_f)T} \left\langle \mathbf{k}_f \,\middle|\, \widehat{U}(T,-T) \,\middle|\, \mathbf{k}_i \right\rangle && \text{(full time-evolution operator)}
\end{aligned}$$

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

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

$\uparrow$

**action**

in discretized form:

$$U\left(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a\right) = \lim_{n\to\infty} C_\epsilon^{n-1} \int d^3x_1 \ldots d^3x_{n-1} \, \exp\left\{ i\epsilon \sum_{k=1}^{n} \left[ \frac{m}{2} \left( \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} \right)^2 - V\left(\mathbf{x}_k\right) \right] \right\}$$

$$\mathbf{x}_0 = \mathbf{x}_a \, , \, \mathbf{x}_n = \mathbf{x}_b \, , \; \epsilon = \frac{t_b - t_a}{n} \longrightarrow 0$$

Convert to **velocity path-integral** by inserting

$$1 = \prod_{k=1}^{n} \int d^3v_k \, \delta\left( \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} - \mathbf{v}_k \right)$$

in the discretized path integral $\Longrightarrow$ all $\mathbf{x}_k$-integrations ($k = 1, \ldots n-1$) can be done

Advantage: boundary conditions included (velocity-integrations unconstrained)

After shift of variables one then obtains

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

with

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

$$\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i \qquad \textbf{momentum transfer}$$

$$\mathbf{K} = \frac{1}{2}\left(\mathbf{k}_i + \mathbf{k}_f\right) \qquad \textbf{mean momentum}$$

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

**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 **??**

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

**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

$$\exp\left(-\frac{i}{4m} T\,\Delta\right) = \int \mathcal{D}^3 w \; \exp\left[-i\int_{-T}^{+T} dt\, \frac{m}{2}\,\mathbf{w}^2(t) \pm \int_{-T}^{+T} dt\, \frac{1}{2}\, f(t)\,\mathbf{w}(t)\cdot\nabla\right]$$

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

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

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

$\uparrow$ impact parameter integral

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

Thus

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

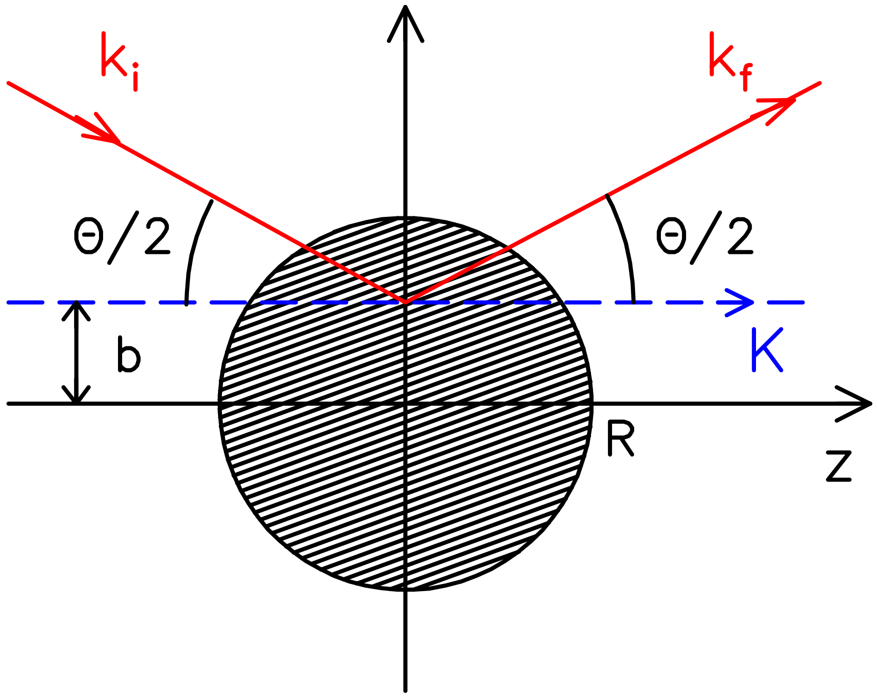
with
$$\boldsymbol{\xi}(t) = \mathbf{b}+\frac{\mathbf{K}}{m}t+\mathbf{x}_v(t)-\mathbf{x}_w(0)$$
$$\dot{\boldsymbol{\xi}}(t) = \frac{\mathbf{K}}{m}+\mathbf{v}(t)$$

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

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

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

with
$$\boldsymbol{\xi}_{\text{ray}}(t) = \mathbf{b}+\frac{\mathbf{p}_{\text{ray}}(t)}{m}t+\mathbf{x}_v(t)-\mathbf{x}_{v\,\perp}(0)-x_w(0)$$
$$\mathbf{p}_{\text{ray}}(t) = \mathbf{K}+\frac{\mathbf{q}}{2}\text{sgn}(t) = \mathbf{k}_i\,\Theta(-t)+\mathbf{k}_f\,\Theta(t)$$




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

# 3. New eikonal expansions

Expect that at high energy and small scattering angle the particle mainly travels along a **straight-line path**.

This is indeed the case: scale

$$t = \frac{m}{K} z \,, \quad \mathbf{v}(t) = \frac{\sqrt{K}}{m} \bar{\mathbf{v}}(z) \,, \quad \mathbf{w}(t) = \frac{\sqrt{K}}{m} \bar{\mathbf{w}}(z)$$

$$\Longrightarrow \quad \mathcal{T}^{(3-3)}_{i \to f} = i \frac{K}{m} \int d^2 b \, e^{-i\mathbf{q}\cdot\mathbf{b}} \int \mathcal{D}^3 \bar{v} \, \mathcal{D}^3 \bar{w} \, \exp \left\{ \frac{i}{2} \int_{-\infty}^{+\infty} dz \, \left[ \bar{\mathbf{v}}^2(z) - \bar{\mathbf{w}}^2(z) \right] \right\}$$

$$\cdot \left\{ \exp \left[ -i \frac{m}{K} \int_{-\infty}^{+\infty} dz \, V \left( \mathbf{b} + \hat{\mathbf{K}} z + \frac{1}{\sqrt{K}} [\mathbf{x}_{\bar{v}}(z) - \mathbf{x}_{\bar{w}}(0)] \right) \right] - 1 \right\}$$

i.e. a **systematic expansion** in powers of $1/K = 1/(k \cos(\theta/2)$ is possible if potential is smooth enough: $KR \gg \left( R \frac{\nabla V}{V} \right)^2 \simeq \left( \frac{R}{a} \right)^2$

$$\mathcal{T}_{i \to f} \simeq i \frac{K}{m} \int d^2 b \, e^{-i\mathbf{q}\cdot\mathbf{b}} \left\{ \exp \left[ i \chi^{(0)}_{AI} + i \chi^{(1)}_{AI} + \ldots \right] - 1 \right\}$$

with

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

**eikonal approximation**

Abarbanel & Itzykson (1969)

$$\chi_{AI}^{(1)}(\mathbf{b}) = \frac{1}{4K}\left(\frac{m}{K}\right)^2\int_{-\infty}^{+\infty} dz_1\, dz_2\, |z_1-z_2|\, \nabla V(\mathbf{b}+\hat{\mathbf{K}}z_1)\cdot\nabla V(\mathbf{b}+\hat{\mathbf{K}}z_2)$$

$\vdots$

**corrections** Wallace (1973)

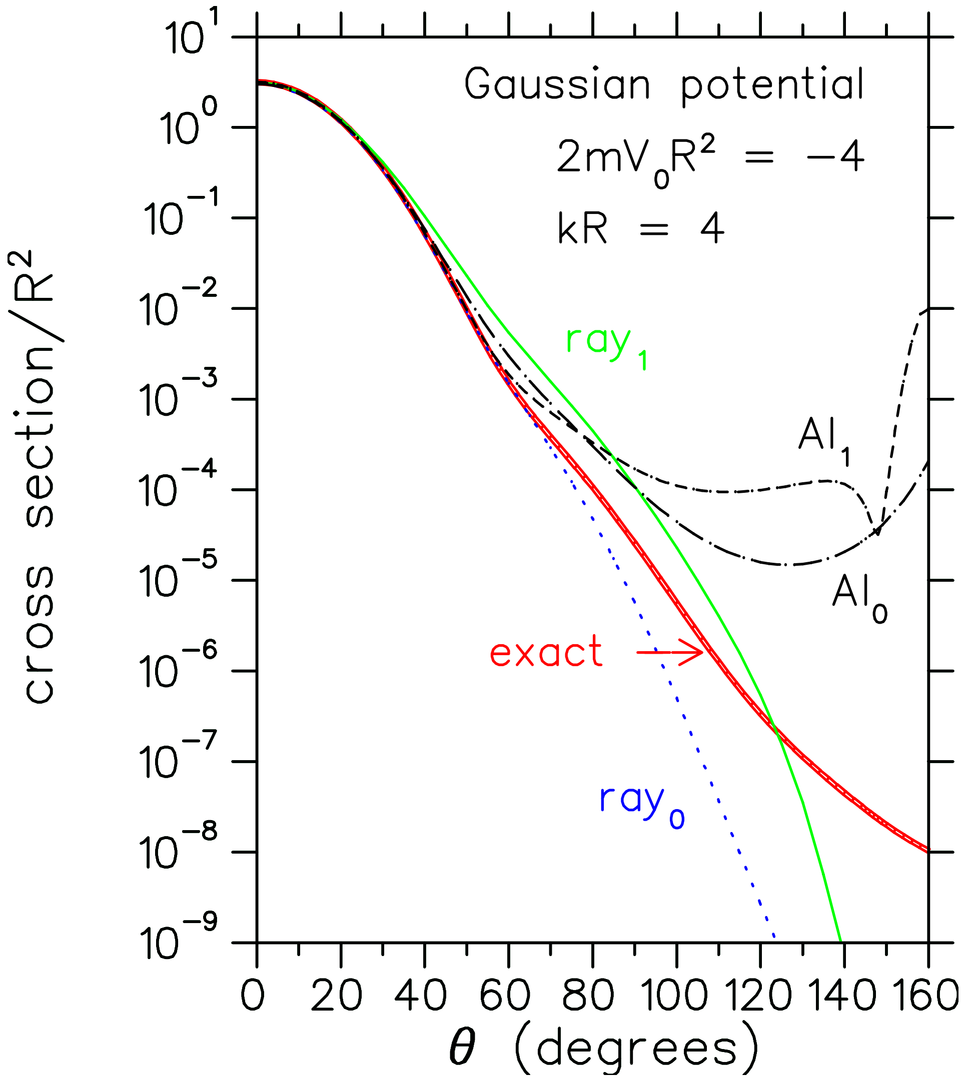
Similarly one obtains a systematic **ray-expansion** by scaling with $1/k$ so that

$$\mathcal{T}_{i\to f} \simeq i\,\frac{K}{m}\int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}}\left\{\exp\left[i\chi_{\rm ray}^{(0)} + i\chi_{\rm ray}^{(1)} - \omega_{\rm ray}^{(1)} + \ldots\right] - 1\right\}$$

with

$$\chi_{\rm ray}^{(0)}(\mathbf{b},\mathbf{q}) = -\frac{m}{k}\int_0^{\infty} dz\, \left[V\left(\mathbf{b}-\hat{\mathbf{k}}_i z\right) + V\left(\mathbf{b}+\hat{\mathbf{k}}_f z\right)\right]$$

$\vdots$


Gaussian potential
$2mV_0R^2 = -4$
$kR = 4$
cross section/$R^2$
$\theta$ (degrees)
$ray_1$
$ray_0$
$AI_1$
$AI_0$
exact
$10^1$
$10^0$
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
$10^{-7}$
$10^{-8}$
$10^{-9}$
0
20
40
60
80
100
120
140
160

# 5. Towards a Monte-Carlo evaluation of high-energy scattering

## Main idea:

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

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

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

$$\exp\left\{ i\,\frac{m}{2}\int dt\,\left[\mathbf{v}(t)^2 - \mathbf{w}(t)^2\right] \right\} \longrightarrow \exp\left\{ -\frac{m}{2}\Gamma \int dt\,\left[\mathbf{v}(t)^2 + \mathbf{w}(t)^2\right] \right\} \cdot \exp\left\{ i\,\frac{m}{2}\int dt\,\left[\mathbf{v}(t)^2 - \mathbf{w}(t)^2\right] \right\}$$

and

$$T^{(\Gamma)}_{i\to f} \longrightarrow \begin{cases} T^{\text{AI}}_{i\to f} & \text{for} \quad \Gamma \to \infty \\ T^{\text{exact}}_{i\to f} & \text{for} \quad \Gamma \to 0 \end{cases}$$

**eikonal approximation built in !**

## **Practical Implementation**:

- Expand velocities in harmonic oscillator wave functions

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

  where $t_0$ is a characteristic time for the scattering process (e.g. $t_0 =$ potential range/velocity)

$$\Longrightarrow \quad \int \mathcal{D}^3 v \mathcal{D}^3 w \longrightarrow \int d^3 v_0 \, d^3 w_0 \, d^3 v_1 \, d^3 w_1 \, \ldots$$

- Evaluate $N$ modes explicitly by **Monte-Carlo integration** with Gaussian weight

$$\exp \left[ -\mathbf{\Gamma} \frac{m}{2} \sum_{n=0}^{N} \left( \mathbf{v}_n^2 + \mathbf{w}_n^2 \right) \right]$$

- Treat the remaining modes (from $N+1$ to $\infty$) by the method of **partial averaging** Doll, Coalson & Freeman (1985) :

$$\int d_{N+1} \ldots d_{\infty} \; e^{\,i\mathcal{A}\,(0\ldots N\,;\,N+1\ldots\infty)} = \int d_{N+1} \ldots d_{\infty} \; \exp\left[\, i(\,\mathcal{A}_t + \underbrace{\mathcal{A} - \mathcal{A}_t}_{=\Delta\mathcal{A}})\,\right]$$

$$= \left( \int d_{N+1} \ldots d_{\infty} \; e^{i\mathcal{A}_t} \right) \cdot \frac{\int d_{N+1} \ldots d_{\infty} \; \exp\left[\, i\mathcal{A}_t\,\right] \exp\left[ i\Delta\mathcal{A}\right]}{\int d_{N+1} \ldots d_{\infty} \; \exp\left[\, i\mathcal{A}_t\,\right]}$$

$$\simeq \left( \int d_{N+1} \ldots d_{\infty} \; e^{i\mathcal{A}_t} \right) \cdot \exp\left\{\, i\; \langle \Delta\mathcal{A} \rangle_{N+1}^{\infty} \,\right\} \;=:\; \exp\left\{\, i\mathcal{A}_{\rm eff}\,(0\ldots N+1)\,\right\}$$

and take for simplicity $\mathcal{A}_t = \mathcal{A}_0$

- Extrapolate the numerical results to $\boldsymbol{\Gamma} = 0$.

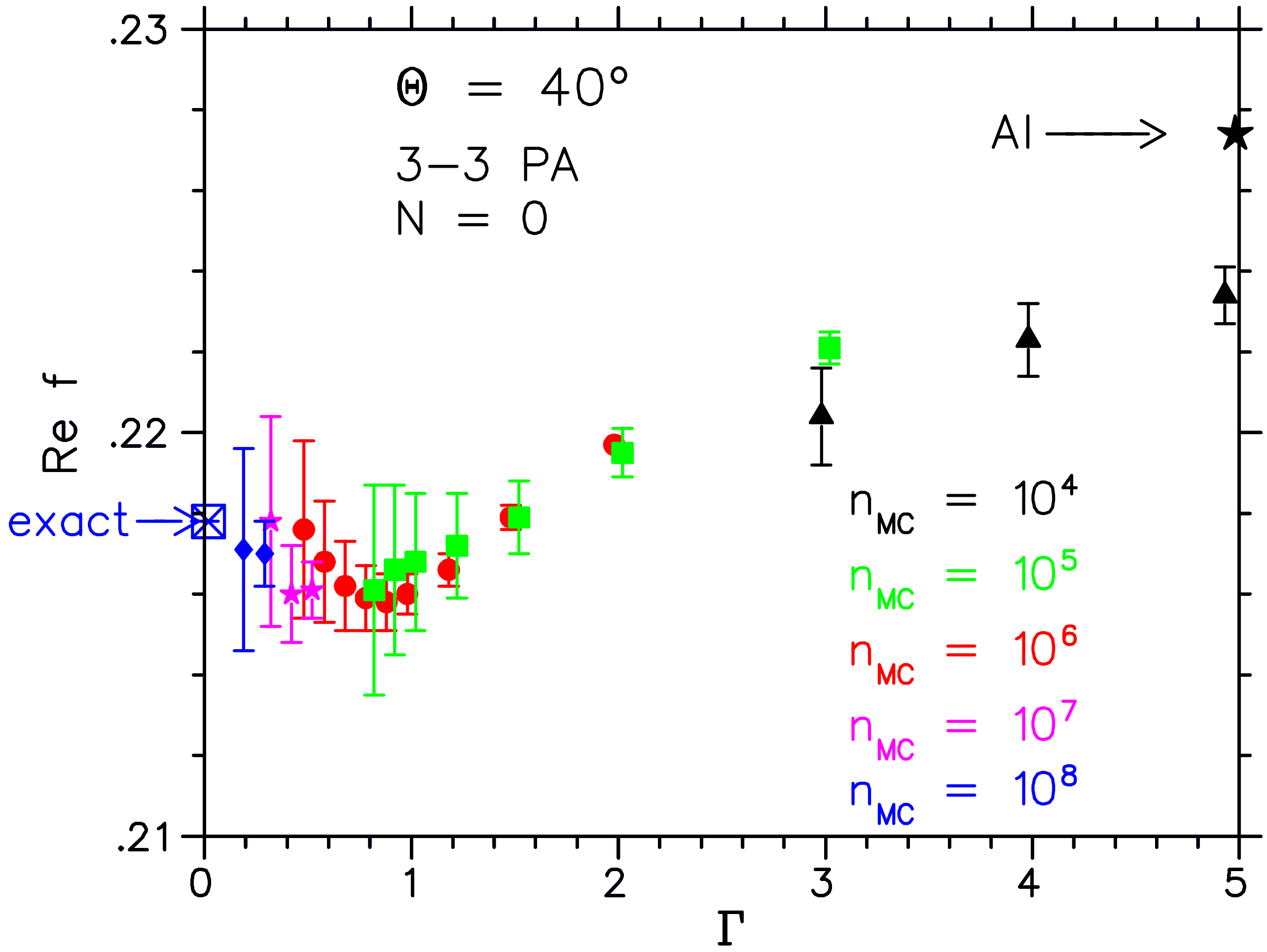
# **Preliminary Results**:

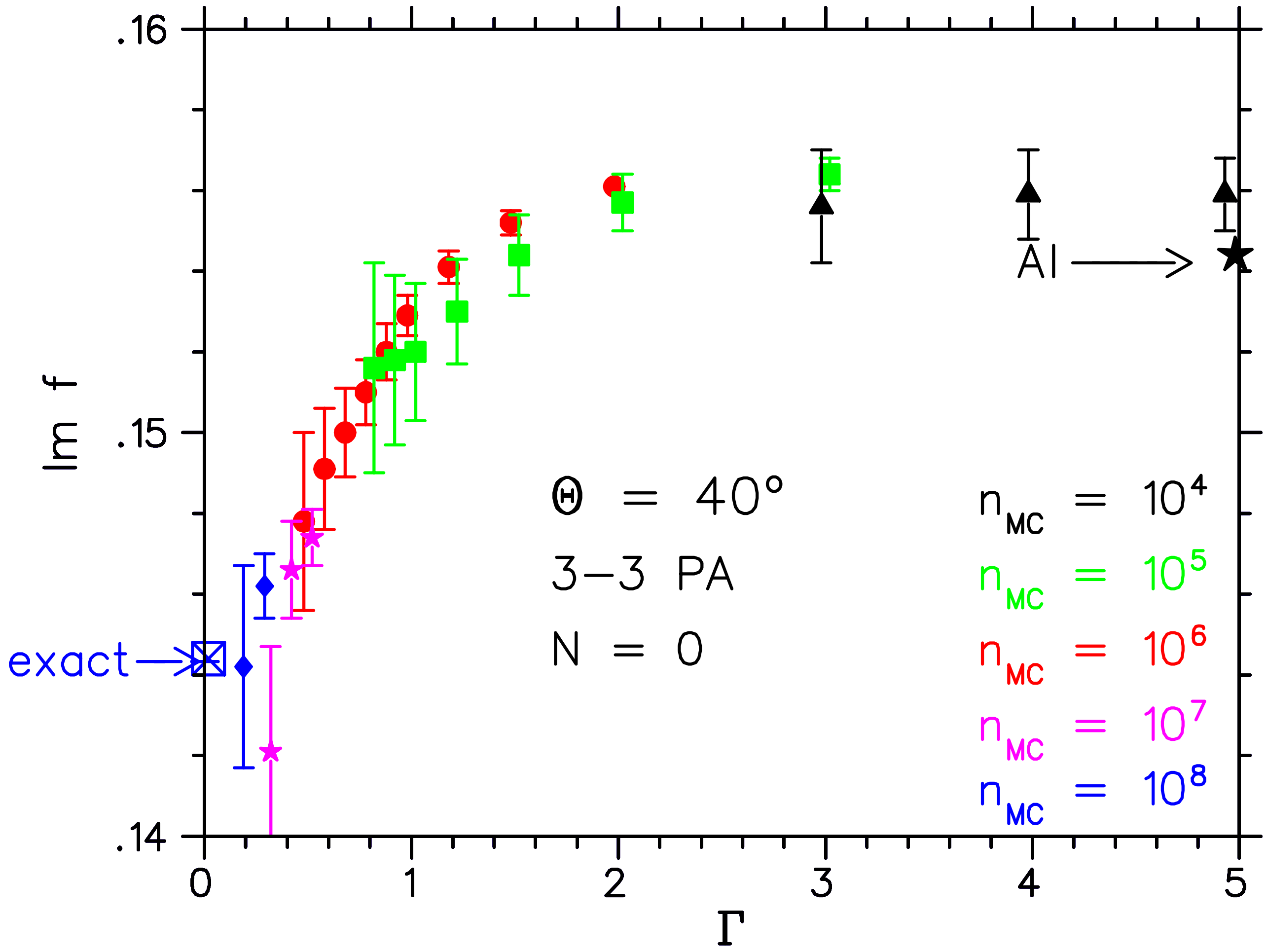
Scattering from a **Gaussian potential**

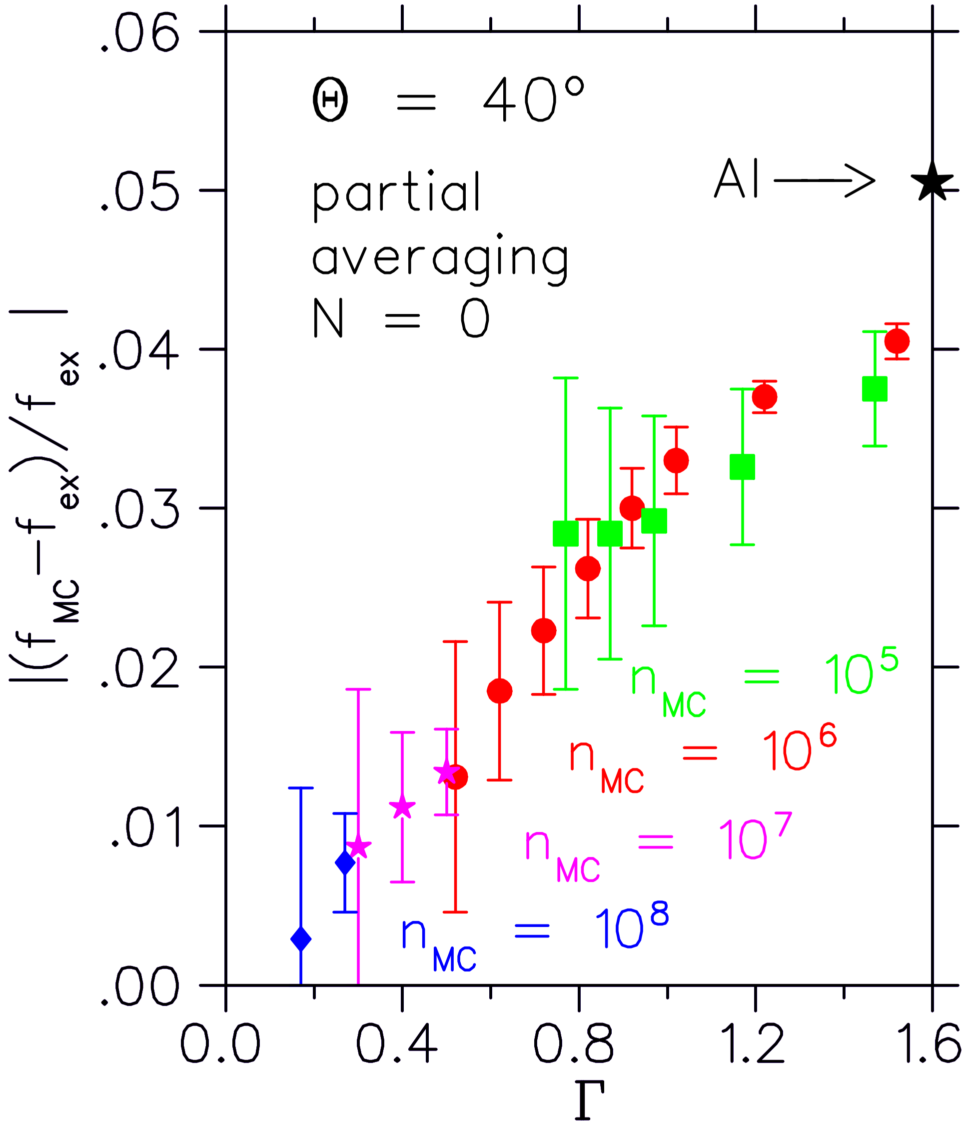
$$V_0 \exp(-r^2/R^2) \qquad \text{with} \;\; kR = 4\,, \quad 2mV_0R^2 = -4$$

Numerical example: $\theta = 40^o, N = 0$. 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.


.23
.22
.21
Re f
exact
Θ = 40°
3–3 PA
N = 0
AI
0
1
2
3
4
5
Γ
n_MC = 10^4
n_MC = 10^5
n_MC = 10^6
n_MC = 10^7
n_MC = 10^8


.16
.15
.14
Im f
0
1
2
3
4
5
Γ
exact
Al
Θ = 40°
3–3 PA
N = 0
$n_{MC} = 10^4$
$n_{MC} = 10^5$
$n_{MC} = 10^6$
$n_{MC} = 10^7$
$n_{MC} = 10^8$


.06
.05
.04
.03
.02
.01
.00
0.0
0.4
0.8
1.2
1.6
Γ
|(f_MC − f_ex)/f_ex|
Θ = 40°
partial
averaging
N = 0
Al ⟶
n_MC = 10^5
n_MC = 10^6
n_MC = 10^7
n_MC = 10^8

# 6. Summary & outlook

- Two **new path integral representations of the $T$-matrix** for non-relativistic potential scattering derived
- Essential ingredients: "**anti-velocity**" to take away phases which would (formally) diverge in the asymptotic limit and **Faddeev-Popov** constraint to factor out energy-conserving $\delta$-function
- Shown to reproduce the **complete Born series** $\longrightarrow$ correct (despite questionable limit procedures ... )
- For high energies these representations give rise to **systematic eikonal-like expansions** and suggest simple **variational approximations**
- First results for **Monte-Carlo evaluation** of high-energy scattering encouraging because eikonal approximation is built in
- Should/could be extended to **multiple scattering** from a many-body target or relativistic scattering