Variational Methods for Path Integral Scattering

J. Carron

Paul-Scherrer Institute, Villigen

April 9, 2009

ETH Master thesis
arXiv:0903.0273

Supervisors : R. Rosenfelder, J. Fröhlich

Outline

Path Integrals for Scattering

The Feynman-Jensen Variational Principle

- A Stationary Expression for the Path Integral.
- Our Ansatz

Analytical Results

- The Approximation in the Eikonal Representation
- The Approximation in the Ray Representation

Numerical Results

The Stage.

- Non-relativistic quantum mechanics.
- Elastic scattering at a potential $V(\mathbf{x})$, vanishing at infinity.
- Incoming and outgoing momenta $\mathbf{k}_i$ and $\mathbf{k}_f$.
- Mean momentum and momentum transfer

$$\mathbf{K} = \frac{1}{2}\left(\mathbf{k}_i + \mathbf{k}_f\right), \quad \mathbf{q} = \mathbf{k}_f - \mathbf{k}_i.$$

Path Integrals for Scattering.

Main Features.

- A phase e^{iS}, S an action, is functionally integrated over two different velocities $\mathbf{v}(t)$,$\mathbf{w}(t)$.
- $\mathbf{w}$: phantom degree of freedom. Removes all seemingly divergent quantities.

  ($\rightarrow$ The kinetic term of $\mathbf{w}$ in the action has the wrong sign).

Path Integrals for Scattering.

Main Features.

- A phase e^{iS}, S an action, is functionally integrated over two different velocities $\mathbf{v}(t)$,$\mathbf{w}(t)$.
- $\mathbf{w}$: phantom degree of freedom. Removes all seemingly divergent quantities.

  ($\rightarrow$ The kinetic term of $\mathbf{w}$ in the action has the wrong sign).
- Interacting part of S: values of the potential are integrated along a one-particle trajectory $\xi(t, \mathbf{v}, \mathbf{w})$.
- The path integral describes the quantum fluctuations around a reference trajectory.

$$\boxed{\rightarrow \xi(t, \mathbf{v}, \mathbf{w}) = \xi_{\rm ref}(t) + \xi_{\rm quant}(t, \mathbf{v}, \mathbf{w}).}$$

The Formulae.

$$T_{i\to f} = i\frac{K}{m}\int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}} \int \mathcal{D}\mathbf{v}\, \mathcal{D}\mathbf{w}\, e^{iS_{\rm free}} \left[e^{i\, S_{\rm int}} - 1 \right] .$$

$$S_{\rm free} = \frac{m}{2}\int dt\, \left[\mathbf{v}^2(t) - \mathbf{w}^2(t) \right] ,$$

$$S_{\rm int} = -\int dt\, V\left(\xi(t)\right), \quad \xi(t) = \xi_{\mathbf{ref}}(t) + \xi_{\mathbf{quant}}(t, \mathbf{v}, \mathbf{w}).$$

The Formulae.

Two Representations.

- Eikonal representation :

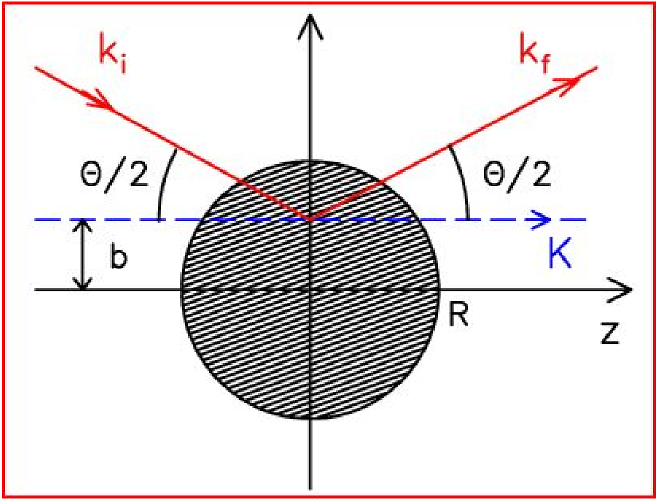
$$\mathbf{w} \text{ 3-dimensional}, \quad \xi_{\mathbf{ref}}(t) = \mathbf{b} + \frac{\mathbf{K}}{m} t.$$

- Ray representation :

$$\mathbf{w} \;\; \| \;\; \mathbf{K}, \quad \xi_{\mathbf{ref}}(t) = \mathbf{b} + \frac{\mathbf{K}}{m} t + \frac{\mathbf{q}}{2m} |t|.$$

In both cases, $\xi_{\mathbf{quant}}(\mathbf{v}, \mathbf{w})$ is linear in the velocities.

Reference Trajectory.



Outline

Path Integrals for Scattering

The Feynman-Jensen Variational Principle
- A Stationary Expression for the Path Integral.
- Our Ansatz

Analytical Results
- The Approximation in the Eikonal Representation
- The Approximation in the Ray Representation

Numerical Results

- Imagine you want to solve a path integral for an action S, knowing its value for another action S_t. You may write

$$\int \mathcal{D}x e^{iS} = \frac{\int \mathcal{D}x \, e^{i(S-S_t)} e^{iS_t}}{\int \mathcal{D}x \, e^{iS_t}} \int \mathcal{D}x e^{iS_t} := \left\langle e^{i(S-S_t)} \right\rangle \int \mathcal{D}x e^{iS_t}.$$

- Imagine you want to solve a path integral for an action S, knowing its value for another action S_t. You may write

$$\int \mathcal{D}x e^{iS} = \frac{\int \mathcal{D}x \; e^{i(S-S_t)} e^{iS_t}}{\int \mathcal{D}x \; e^{iS_t}} \int \mathcal{D}x e^{iS_t} := \left\langle e^{i(S-S_t)} \right\rangle \int \mathcal{D}x e^{iS_t}.$$

- Consider in place of the above expression the following functional:

$$\boxed{F[S_t] = e^{i\langle S-S_t \rangle} \int \mathcal{D}x \; e^{iS_t}}.$$

- Imagine you want to solve a path integral for an action S, knowing its value for another action S_t. You may write

$$\int \mathcal{D}x e^{iS} = \frac{\int \mathcal{D}x\, e^{i(S-S_t)} e^{iS_t}}{\int \mathcal{D}x\, e^{iS_t}} \int \mathcal{D}x e^{iS_t} := \left\langle e^{i(S-S_t)} \right\rangle \int \mathcal{D}x e^{iS_t}.$$

- Consider in place of the above expression the following functional:

$$\boxed{F[S_t] = e^{i\langle S-S_t\rangle} \int \mathcal{D}x\, e^{iS_t}}.$$

- It holds that

$$F[S] = \int \mathcal{D}x\, e^{iS} \quad \text{and} \quad \delta F|_{S=S_t} = 0.$$

- Imagine you want to solve a path integral for an action S, knowing its value for another action S_t. You may write

$$\int \mathcal{D}x e^{iS} = \frac{\int \mathcal{D}x\ e^{i(S-S_t)} e^{iS_t}}{\int \mathcal{D}x\ e^{iS_t}} \int \mathcal{D}x e^{iS_t} := \left\langle e^{i(S-S_t)} \right\rangle \int \mathcal{D}x e^{iS_t}.$$

- Consider in place of the above expression the following functional:

$$\boxed{F[S_t] = e^{i\langle S-S_t\rangle} \int \mathcal{D}x\ e^{iS_t}}.$$

- It holds that

$$F[S] = \int \mathcal{D}x\ e^{iS} \quad \text{and} \quad \delta F|_{S=S_t} = 0.$$

- We have thus found a stationary expression for the path integral, which we can solve for a nearby action S_t.

Corrections.

Two ways to expand $\left\langle e^{it\Delta S}\right\rangle$:

- Expansion in moments :

$$\left\langle e^{it\Delta S}\right\rangle = \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \left\langle (\Delta S)^k \right\rangle .$$

- Expansion in cumulants λ_k:

$$\left\langle e^{it\Delta S}\right\rangle := \exp\left[\sum_{k=1}^{\infty} \frac{(it)^k}{k!} \lambda_k\right] .$$

$$\Rightarrow \lambda_1 = \langle \Delta S \rangle , \quad \lambda_2 = \left\langle (\Delta S)^2 \right\rangle - \langle \Delta S \rangle^2$$

Corrections.

Two ways to expand $\langle e^{it\Delta S}\rangle$:

- Expansion in moments :

$$\left\langle e^{it\Delta S}\right\rangle = \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \left\langle (\Delta S)^k \right\rangle .$$

- Expansion in cumulants λ_k:

$$\left\langle e^{it\Delta S}\right\rangle := \exp\left[\sum_{k=1}^{\infty} \frac{(it)^k}{k!}\lambda_k\right] .$$

$$\Rightarrow \lambda_1 = \langle \Delta S\rangle , \quad \lambda_2 = \left\langle (\Delta S)^2 \right\rangle - \langle \Delta S\rangle^2$$

- Our variational approximation is the first term of the cumulant expansion.
- The first correction term is given by $F[S_t] \to F[S_t] \exp\left(-\frac{1}{2}\lambda_2\right)$.

Outline

Path Integrals for Scattering

The Feynman-Jensen Variational Principle
- A Stationary Expression for the Path Integral.
- Our Ansatz

Analytical Results
- The Approximation in the Eikonal Representation
- The Approximation in the Ray Representation

Numerical Results

Which Trial Action ?

The trial action S_t has to satisfy two criteria:

1. It must have a physical motivation.
2. It must be simple enough to allow analytical calculations. (very restrictive !)

Our Ansatz I.

Motivation:

- In a high-energy approach to our path integral, one would expand the interacting part of the action in

$$V(\xi_{\mathbf{ref}} + \xi_{\mathbf{quant}}(\mathbf{v}, \mathbf{w})) \approx V(\xi_{\mathbf{ref}}) + \nabla V(\xi_{\mathbf{ref}}) \cdot \xi_{\mathbf{quant}}(\mathbf{v}, \mathbf{w}).$$

- This makes the interacting part of the action linear in the velocities ($\rightarrow$ leads to eikonal-like expansions).

Our Ansatz II.

This suggests:

- Our Ansatz will be to add to the free action a linear term in the velocities.
- The variational procedure will pick up for us the best linear term possible, while emulating the structure of the high-energy expansion.

What we do.

In our path integral formulae for the T-Matrix, instead of

$$\int \mathcal{D}\mathbf{v}\mathcal{D}\mathbf{w}\ e^{iS},$$

we will therefore consider

$$F[S_t] = e^{i\langle S - S_t\rangle} \int \mathcal{D}\mathbf{v}\mathcal{D}\mathbf{w}\ e^{iS_t},$$

where the trial action is linear in the velocities,

$$\rightarrow S_t = S_{\text{free}} + \int dt\, \mathbf{B}(t)\cdot\mathbf{v}(t) + \int dt\, \mathbf{C}(t)\cdot\mathbf{w}(t)$$

Expectations.

The problem is reduced to:

1. The computation of the needed expectation values.
2. The solution to the variational equations for $\mathbf{B}(t)$ and $\mathbf{C}(t)$ arising from the stationarity condition.

Expectations.

The problem is reduced to:

1. The computation of the needed expectation values.
2. The solution to the variational equations for $\mathbf{B}(t)$ and $\mathbf{C}(t)$ arising from the stationarity condition.

We expect:

1. To recover in the high-energy limit (at least) the leading and next-to-leading term of the eikonal expansion.
2. That the approximation should also be valid for lower energies or larger scattering angles.

Results Valid in both Representations.

Results Valid in both Representations.

- In both representations, the variational approximation results
  in two scattering phases, $X_0 \propto V$ and $X_1 \propto V^2$.

$$\rightarrow T_{i\rightarrow f} \sim \int d^2b \, e^{-i\mathbf{q}\cdot\mathbf{b}} \left[e^{i(X_0+X_1)} - 1 \right].$$

- The introduction of the linear term in the action leads to a new trajectory, which we call now $\mathbf{x}(t)$.
- All the information is contained in this variational trajectory, which is given in integral form.
  (one may forget about **B** *and* **C**).

Outline

Path Integrals for Scattering

The Feynman-Jensen Variational Principle
- A Stationary Expression for the Path Integral.
- Our Ansatz

Analytical Results
- The Approximation in the Eikonal Representation
- The Approximation in the Ray Representation

Numerical Results

The Scattering Phases.

- In the eikonal representation, the scattering phases are

$$X_0 = -\int dt\, V(\mathbf{x}(t))$$

and

$$X_1 = -\frac{1}{4m}\int dt \int ds\, \nabla V(\mathbf{x}(t)) \cdot \nabla V(\mathbf{x}(s)) |t - s| .$$

- These are identical to the first two phases of the eikonal expansion (Wallace 1971), expect for
  - the replacement of $\mathbf{b} + \frac{\mathbf{K}}{m} t$ with $\mathbf{x}(t)$,
  - the minus sign in front of X_1.

The Variational Trajectory.

- The variational trajectory is given by

$$\mathbf{x}(t) = \mathbf{b} + \frac{\mathbf{K}}{m}t - \frac{1}{2m}\int ds\, \nabla V(\mathbf{x}(s))|t-s|.$$

- By differentiating twice,

The Variational Trajectory.

- The variational trajectory is given by

$$\mathbf{x}(t) = \mathbf{b} + \frac{\mathbf{K}}{m}t - \frac{1}{2m}\int ds\,\nabla V(\mathbf{x}(s))|t-s|.$$

- By differentiating twice,

$$\ddot{\mathbf{x}}(t) = -\frac{1}{m}\nabla V(\mathbf{x}(t)).$$

The Variational Trajectory II.

This integral equation

$$\mathbf{x}(t) = \mathbf{b} + \frac{\mathbf{K}}{m} t - \frac{1}{2m} \int ds \, \nabla V(\mathbf{x}(s)) |t - s|,$$

- is the classical analogue of the Lippman-Schwinger wave equation,
- it describes a classical scattering process with mean momentum **K**.

Behaviour at High Energy.

One expands in inverse powers of the incoming momentum k, while holding m/k constant:

- The variational trajectory, and the scattering phases X_0 and X_1.
- The factors of

$$K = k\sqrt{1 - \frac{q^2}{4k^2}}.$$

The result can be compared to the systematic eikonal expansion, given by

$$T_{i\to f} \sim \int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}} \left[e^{i\chi_0 + i\chi_1 + i\chi_2 - \omega_2 + \cdots} \right]$$

Behaviour at High Energy II.

One finds that the variational approximation contains

- the leading term,
- the first order correction (with the correct sign...),

Behaviour at High Energy II.

One finds that the variational approximation contains

- the leading term,
- the first order correction (with the correct sign...),
- as well as the imaginary part of the second order term.

$$T_{i\to f}^{\text{variational}} \longrightarrow \int d^2b\, e^{-i\mathbf{q}\cdot\mathbf{b}} \left[e^{i\chi_0 + i\chi_1 + i\chi_2 + \cdots} \right]$$

Note on the second cumulant.

- The second cumulant is also given in integrating values of potential derivatives along this variational trajectory.
- It completes the real part of the second order term ω_2, and parts of higher order terms.

Outline

Path Integrals for Scattering

The Feynman-Jensen Variational Principle
- A Stationary Expression for the Path Integral.
- Our Ansatz

Analytical Results
- The Approximation in the Eikonal Representation
- The Approximation in the Ray Representation

Numerical Results

The Ray Scattering Phases.

- In the ray representation, the scattering phases are

$$X_0 = -\int dt\ V_{\sigma(t)}(\mathbf{x}(t))$$

and

$$X_1 = -\frac{1}{4m}\int dt ds \nabla V_{\sigma(t)}(\mathbf{x}(t)) \cdot \nabla V_{\sigma(s)}(\mathbf{x}(s)) \left[|t-s| - |t| - |s| \right].$$

- These are similar to the phases in the eikonal representation. However,
  - these are complex quantities,
  - the potential V is replaced by a new, effective potential V_σ,
  - the variational trajectory shows now some different properties.

Effective Potential.

- This new potential is defined in Fourier space as the Gauss transformation

$$\widetilde{V}_{\sigma(t)}(\mathbf{p}) := \widetilde{V}(\mathbf{p}) \exp\left(-i|t|\frac{\mathbf{p}_{\perp}^2}{2m}\right).$$

- It is a complex quantity.
- It takes some quantum mechanical aspects into account.

The Ray Variational Trajectory.

- The variational trajectory is given by

$$\mathbf{x}(t) = \mathbf{b} + \frac{\mathbf{K}}{m} t + \frac{\mathbf{q}}{2m} |t| - \frac{1}{2m} \int ds \nabla V_{\sigma(s)}(\mathbf{x}(s)) \left[|t-s| - |t| - |s| \right].$$

The Ray Variational Trajectory.

- The variational trajectory is given by

$$\mathbf{x}(t) = \mathbf{b} + \frac{\mathbf{K}}{m} t + \frac{\mathbf{q}}{2m} |t| - \frac{1}{2m} \int ds \nabla V_{\sigma(s)}(\mathbf{x}(s)) \left[|t-s| - |t| - |s| \right].$$

- By differentiating twice,

$$m\,\ddot{\mathbf{x}}(t) = -\nabla V_{\sigma(t)}(\mathbf{x}(t)) + \delta(t) \left(\mathbf{q} + \int ds\, \nabla V_{\sigma(s)}(\mathbf{x}(s)) \right).$$

- It describes thus a (complex...) classical scattering trajectory, except a time $t = 0$, when it suffers a kick.

The Ray Variational Trajectory II.

- Asymptotics: For large $|t|$,

$$|t - s| - |t| - |s| \to \text{independent of } t.$$

- It follows that at $\pm$ infinity,

$$\dot{\mathbf{x}}(t) = \frac{\mathbf{K}}{m} \pm \frac{\mathbf{q}}{2m}.$$

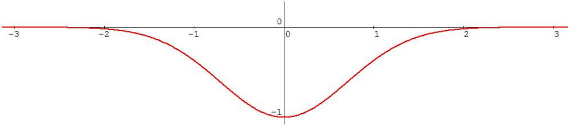
- Especially, **K** and **q** have in this classical trajectory the same meaning of mean momentum and momentum transfer.

Numerical Results.

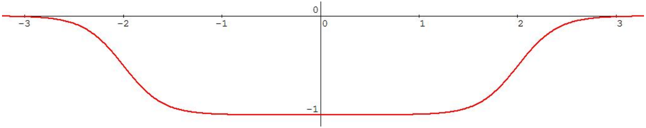
Numerical Results.

We tested the accuracy of the approximation for two particular potentials,

- Gaussian,



- Woods-Saxon,



with parameters corresponding to an high-energy situation in nuclear physics where the eikonal approximation was previously found unsatisfactory.

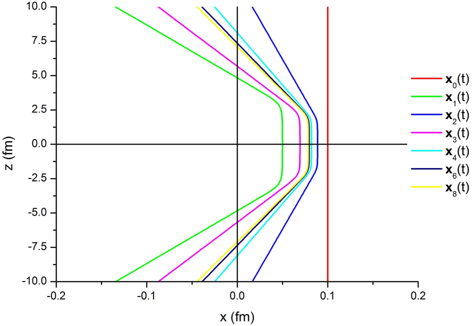
The trajectories were obtained through iteration:

$$\begin{aligned} \mathbf{x}_{n+1}(t) &= \mathbf{b} + \frac{\mathbf{K}}{m}t - \frac{1}{2m}\int ds\, \nabla V(\mathbf{x}_n(s))|t-s|, \\ \mathbf{x}_0(t) &= \mathbf{b} + \frac{\mathbf{K}}{m}t. \end{aligned}$$

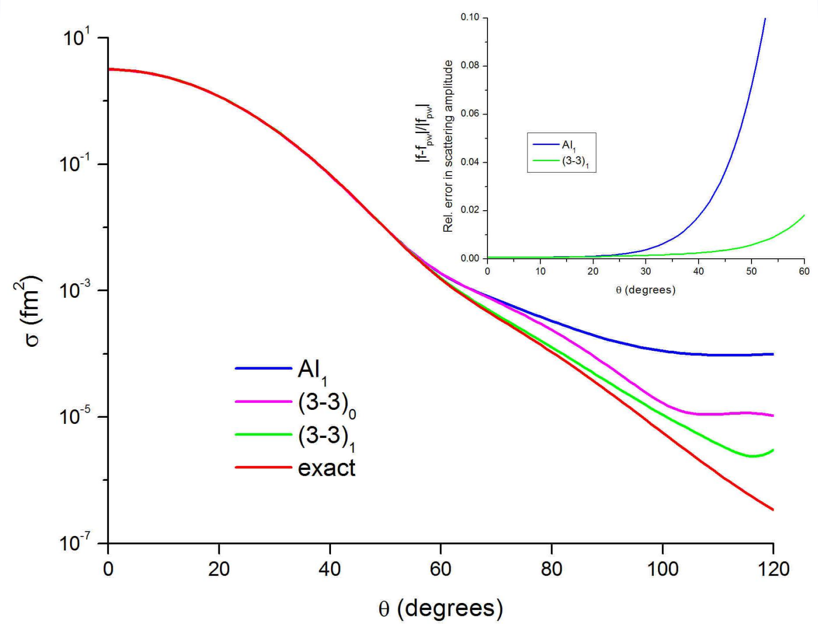
The trajectories were obtained through iteration:

$$\mathbf{x}_{n+1}(t) = \mathbf{b} + \frac{\mathbf{K}}{m}t - \frac{1}{2m}\int ds\, \nabla V(\mathbf{x}_n(s))|t-s|,$$

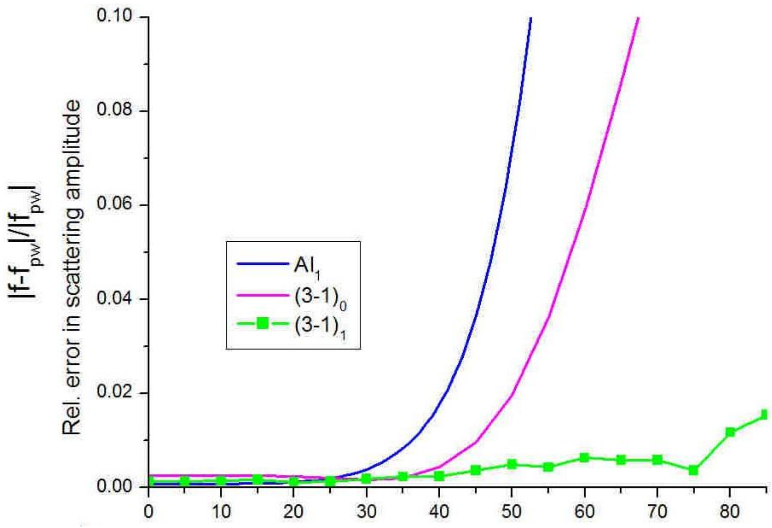
$$\mathbf{x}_0(t) = \mathbf{b} + \frac{\mathbf{K}}{m}t.$$



- Integrations were performed with the Gauss-Legendre rule, except for the second cumulant, where an adaptive integration scheme was used.
- Oscillatory character of the second cumulant very annoying...



10^1
10^{-1}
10^{-3}
10^{-5}
10^{-7}
σ (fm²)
0
20
40
60
80
100
120
θ (degrees)
Al₁
(3-3)₀
(3-3)₁
exact
|f-f_pw|/|f_pw|
Rel. error in scattering amplitude
0.00
0.02
0.04
0.06
0.08
0.10
0
10
20
30
40
50
60
θ (degrees)
Al₁
(3-3)₁


|f-f_pw|/|f_pw|
Rel. error in scattering amplitude
0.10
0.08
0.06
0.04
0.02
0.00
0
10
20
30
40
50
60
70
80
AI_1
(3-1)_0
(3-1)_1

Outlook

Now

- The most general quadratic Ansatz can also be investigated.
- The scattering process is then described by the same variational trajectory, with the potential

$$\widetilde{V}_{\sigma(t)}(\mathbf{p}) = \widetilde{V}(\mathbf{p}) \exp\left(-\frac{i}{2}\mathbf{p}^T \cdot \sigma(t)\mathbf{p}\right).$$

- $\sigma(t)$ is now a matrix, that satisfies also a "Lippmann-Schwinger" equation

$$\sigma = \sigma_0 + \sigma H \sigma_0, \quad H_{ij} \equiv \partial_i \partial_j V_\sigma,$$

σ_0 "free classical propagator".

Outlook

Longer Term

- This variational approximation could play a role in the stochastic evaluation of the scattering process.
- Multibody scattering.

Summary

- We have investigated a completely new way to address the scattering process.
- Singles out one particle classical trajectories, evolving according to an effective potential.
- Rather accurate.

Low-energy behaviour ???