S-scattering in a spherical potential:

Simple and instructive example of Bold Diagrammatic Monte Carlo

Prokof'ev, and Svistunov, *Bold Diagrammatic Monte Carlo Technique: When Sign Problem is Welcome*, PRL 99, 250201 (2007).

Consider the following problem: Find f defined by the series $(u > 0)$:

$$f = a - au + au^2 - au^3 + \ldots + a(-1)^n u^n + \ldots = a\sum_{n=0}^{\infty}(-1)^n u^n = \frac{a}{1+u}$$

Do it my Monte Carlo assuming that the answer in blue is not known.
Consider this as "diagrams" characterized only by the diagram "order" , i.e.

$$\nu = n, \quad D_\nu = au^n, \quad A_\nu = (-1)^n, \quad f = \langle A \rangle = \sum_\nu A_\nu D_\nu$$

Monte carlo Algorithm: **one update** $n \leftrightarrow n \pm 1$ (decide at random + or -)

Detailed balance equation: $D_n \frac{1}{2} P_{n \to n\pm1} = D_{n\pm1} \frac{1}{2} P_{n\pm1 \to n}$

$$R = \frac{P_{n\to n+1}}{P_{n+1\to n}} = u, \qquad R = \frac{P_{n\to n-1}}{P_{n-1\to n}} = \frac{1}{u} \quad \text{(reject if n=0)}$$

This is all! $f^{(MC)} = f^{(MC)} + (-1)^n, \quad Z = Z + \delta_{n,0}, \quad f = a\frac{f^{(MC)}}{Z}$

Solving self-consistent equations using Diag.MC

$$f = a - uf$$

$$f = \frac{a}{1+u}$$

use Diag.MC

MC scheme
each diagram → f

$$f_{n+1} = a - u\langle f \rangle_{MC,n}$$

$$\langle f \rangle_{MC,n} = \sum_{i=1}^{n} \frac{f_i}{n}$$

$$f_{n+1} = a - u\sum_{i=1}^{n} \frac{f_i}{n}$$

solve it iteratively

$f_0=a$
$f_{n+1}=a-uf_n$

⇩

$f_0=a$
$f_1=a-uf_0=a-ua$
$f_2=a-uf_1=a-ua+u^2a$
…….

$f=a-ua+u^2a-u^3a+u^4a- \cdots$

|u|>1, divergent series:
resummation techniques

Write a simple program which mimicks a Monte Carlo calculation

$a = 1$ $\quad u = 2.5$

$f_1 = a$

do loop

$$f_{n+1} = a - u \sum_{i=1}^{n} \frac{f_i}{n}$$

end do loop

→

1	1.
2	-1.5
3	1.625
4	0.0625
5	0.2578125
6	0.27734375
7	0.282226562
8	0.283970424
9	0.284733364
10	0.285114833
11	0.285324642
12	0.285448619
13	0.285526105
14	0.285576769
15	0.285611148
16	0.285635214
17	0.285652511
18	0.285665229
19	0.285674768
20	0.285682048

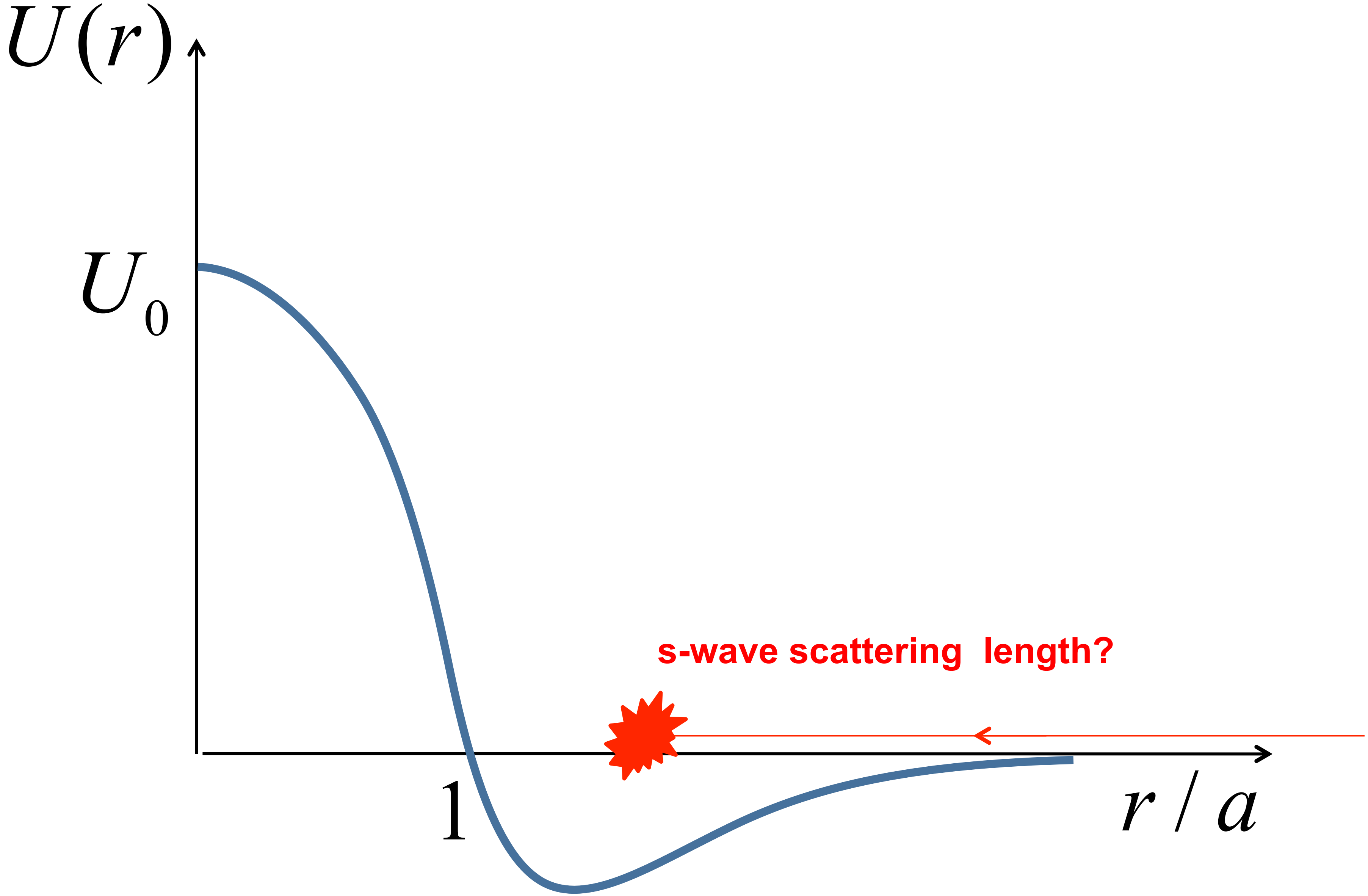
f=0.285714286

```
double precision:: a=1.0,  u=2.5
double precision:: f_new, f_sum
integer :: n=20,i

f_sum = a

do i = 1, n
     print*, i, f_new
   f_new = a – u * f_sum/i
   f_sum = f_sum + f_new
enddo

print*, f_new
end
```



$U(r)$
U_0
s-wave scattering length?
1
r/a

$$f(q) = -u(q) - (1/\pi)\int_{-1}^{1} d\chi \int_{0}^{\infty} u\left(|\mathbf{q}-\mathbf{q}_1|\right) f(q_1)\, dq_1$$

S-scattering wavefunction

$$|\mathbf{q}-\mathbf{q}_1| \equiv \sqrt{q^2 + q_1^2 - 2qq_1\chi}$$

$$u(q) = (1/\pi)\int U\left(r\right) \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}}\, d^3 r$$

Spherically symmetric potential

$a = -f(0)$ S-scattering length: the quantity of interest

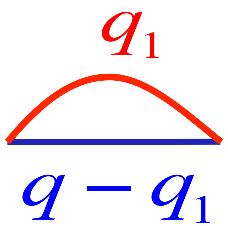
Generic

$$Q(y) = \sum_{m=0}^{\infty} \sum_{\xi_m} \int D(\xi_m, y, x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m$$

Our case

$$f(q) = D_1(q) + \int_{-1}^{1} d\chi \int_0^{\infty} dq_1\; D_2(q, q_1, \chi)$$

$$D_1(q) = -u(q)$$



$$D_2(q, q_1, \chi) = -\,(1/\pi)\, u\left(\sqrt{q^2 + q_1^2 - 2 q q_1 \chi}\right) f(q_1)$$

Generic

$$R_A\left(\vec{X}\right) = \frac{New\ Diagram}{Old\ Diagram}\,\frac{1}{\Omega\left(\vec{X}\right)}$$

$\Omega\left(\vec{X}\right)$ *is an **arbitrary** distribution function for generating particular values of new continuous variables in the update A .*

$$R_B\left(\vec{X}\right) = \frac{New\ Diagram}{Old\ Diagram}\,\Omega\left(\vec{X}\right)$$

Our case

$$R_{1\to 2} = \frac{(1/\pi)\left|u\left(\sqrt{q^2+q_1^2-2qq_1\chi}\right)f(q_1)\right|}{|u(q)|}\,\frac{p_2/p_1}{\Omega_\chi(\chi)\,\Omega_q(q_1)}$$

$$R_{2\to 1} = \frac{|u(q)|}{(1/\pi)\left|u\left(\sqrt{q^2+q_1^2-2qq_1\chi}\right)f(q_1)\right|}\,\frac{\Omega_\chi(\chi)\,\Omega_q(q_1)}{p_2/p_1}$$

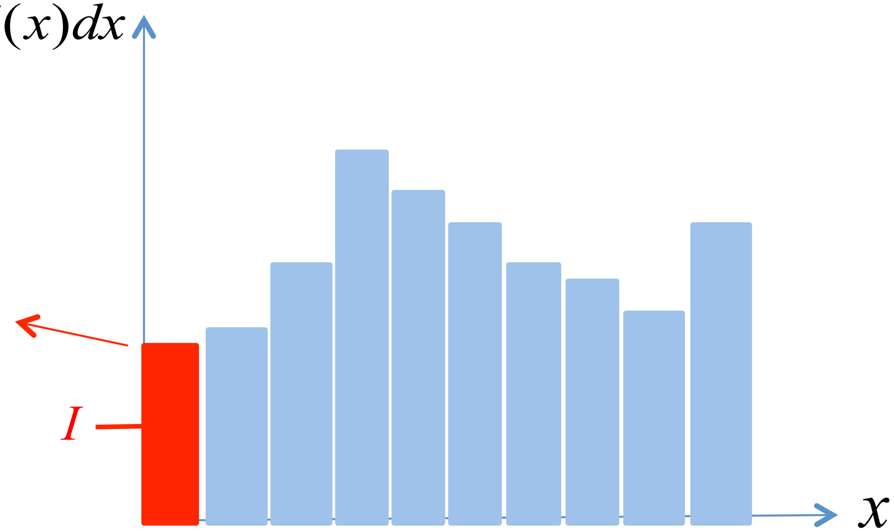
Normalization:

histogram $h_{bin} \propto \int_{bin} f(x)dx$

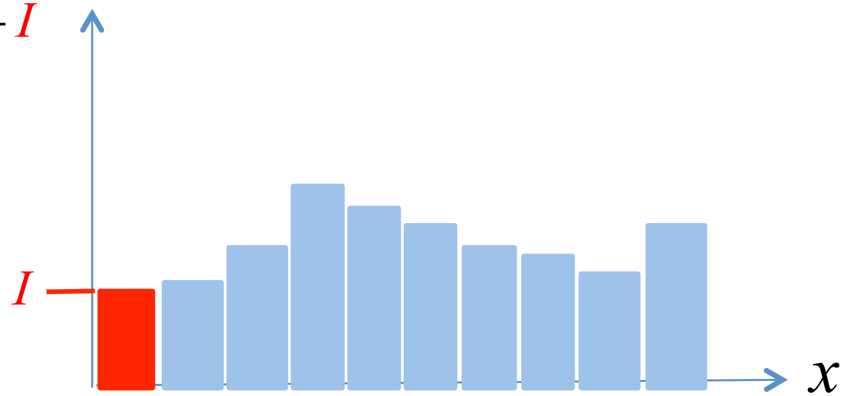
special "bin" where

$$\int_{bin} f(x)dx = I$$

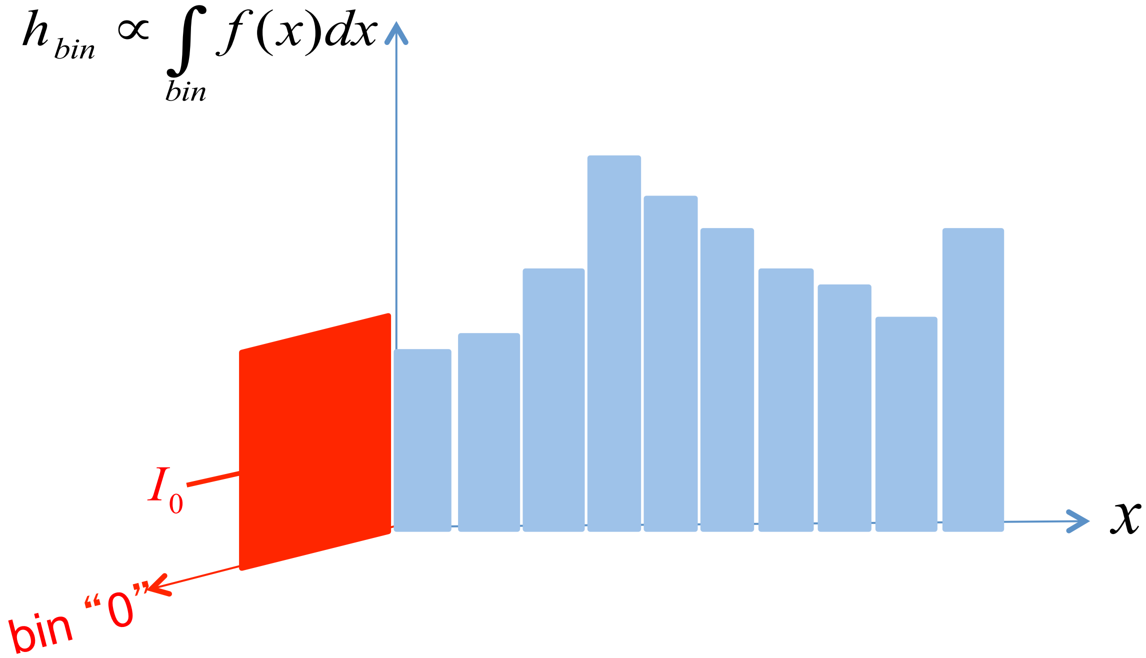
is known exactly

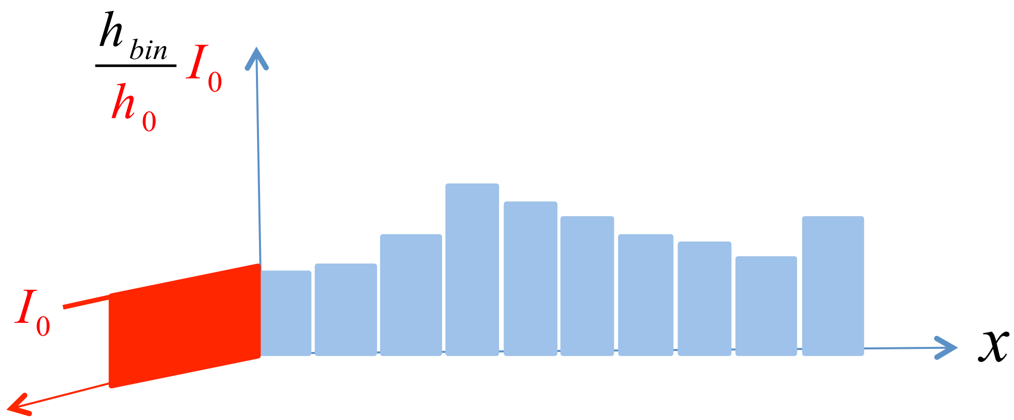


Normalized histogram $\frac{h_{bin}}{h_{sbin}} I$



Normalization using “desined bin”:





Normalization

$$I = \int |u(q)|\, dq + (1/\pi)\int d\chi \int dq \int dq_1 \left| u\left(\sqrt{q^2 + q_1^2 - 2qq_1\chi}\right) f(q_1) \right|$$

global partition function
(drops out from final Eqs.)

$$I_u = \int |u(q)|\, dq$$

number of 1-type diagrams in the MC statistics

sum of all contributions
to the s-th bin of the histogram

$$\frac{Z_1}{Z_{\rm MC}} \to \frac{I_u}{I} \qquad\qquad \frac{H_s}{Z_{\rm MC}} \to I^{-1} \int_{\text{bin}\_s} f(q)\, dq$$

number of MC steps (= total number of diagrams in the MC statistics)

$$I = \frac{Z_{\rm MC}}{Z_1} I_u \quad \Rightarrow \quad \boxed{\int_{\text{bin}\_s} f(q)\, dq \leftarrow \frac{I_u}{Z_1} H_s}$$

$\rightarrow$ reads '***approaches in the statistical limit***'

$\leftarrow$ reads '***being estimated as***'

Normalization via a special non-physical diagram

Introduce a special (non-physical) normalization diagram D_0 which is just a number (not a function). Sample the three diagrams, 0, 1, and 2 through the updates $1 \rightleftarrows 2$ (same as before) and $0 \rightleftarrows 1$ (new update).

$$R_{0\to 1} = \frac{|u(q)|}{D_0} \frac{p_1 / p_0}{\Omega_q(q)} \qquad\qquad R_{1\to 0} = \frac{D_0}{|u(q)|} \frac{\Omega_q(q)}{p_1 / p_0}$$

$$\tilde{I} = D_0 + \int |u(q)| dq + (1/\pi) \int d\chi \int dq \int dq_1 \left| u\left(\sqrt{q^2 + q_1^2 - 2qq_1\chi}\right) f(q_1) \right|$$

modified g
partition f

number of normalization diagrams in the MC statistics

$$\frac{Z_0}{Z_{MC}} \to \frac{D_0}{\tilde{I}} \qquad\qquad \frac{H_s}{Z_{MC}} \to \tilde{I}^{-1} \int_{\text{bin\_s}} f(q) dq$$

$$\tilde{I} = \frac{Z_{MC}}{Z} D_0 \quad \Rightarrow \quad \int f(q) dq \leftarrow \frac{D_0}{Z} H_s$$

Example of a solution (attractive ‘square’ potential well)