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).

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

S-scattering wavefunction

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

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

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

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

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

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

Our case

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

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

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

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

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

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

$\to$ reads ‘***approaches in the statistical limit***’

$\leftarrow$ reads ‘***being estimated as***’

Estimator for s-scattering length

$$a = u(0) + (2/\pi)\int u(q)f(q)dq \leftarrow u(0) + (2/\pi)\frac{I_u}{Z_1}\sum_s u(q_s)H_s$$

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).

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

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

modified global partition function

number of normalization diagrams in the MC statistics

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

$$\tilde{I} = \frac{Z_{\mathrm{MC}}}{Z_0} D_0 \quad \Rightarrow \quad \boxed{\int_{\mathrm{bin\_}s} f(q)\,dq \leftarrow \frac{D_0}{Z_0} H_s}$$

Estimator for s-scattering length

$$a = u(0) + (2/\pi)\int u(q)f(q)dq \leftarrow u(0) + (2/\pi)\frac{D_0}{Z_0}\sum_s u(q_s)H_s$$

Example of a solution (attractive 'square' potential well)