# NATO Advanced Study Institute: Quantum Monte Carlo Methods in Physics and Chemistry. Workshop Exercises


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## I. PARTICLE IN A TWO-DIMENSIONAL BOX

Use correlated Monte Carlo to find the antisymmetric solution of the Schroedinger equation for a particle in a square with hard walls. Follow the method outlined in Liu, Zhang, and Kalos, Phys. Rev. E, Vol 50, p 3220 (1994), sections I and II

## II. ONE-DIMENSIONAL HARMONIC OSCILLATOR: 1

Solve the Schroedinger equation to find the first antisymmetric state of the one-dimensional harmonic oscillator, following the method in Kalos and Schmidt, J. Stat. Phys., Vol 89, p 425 (1997). Use the exact form of the Green's function with $\tau = 0.1$, and an equal mix of "reflected" and "parallel" dynamics. Record in histograms the distributions of positive and negative walkers and the difference. Comment on the way in which the "plus-minus" symmetry is broken. Obtain an eigenvalue using the "projection" or "test" function

$$\psi_T(x) = e^{-(x-x_0)^2/2} - e^{-(x+x_0)^2/2} \tag{2.1}$$

with $x_0 = 0.25$.

## III. ONE-DIMENSIONAL HARMONIC OSCILLATOR: 2

Solve the Schroedinger equation to find the first antisymmetric state of the one-dimensional harmonic oscillator, following the method given in the second lecture: Use simple diffusion Monte Carlo with different importance or "guiding" functions for positive and negative walkers:

$$\psi_G^{\pm} = e^{-x^2/2}\sqrt{(1+(c*x)^2)} \pm cx \tag{3.1}$$

for $c = 0.01$. Use simple cancellation of the walkers using the Gaussian kernel. Use the same $\psi_T(x)$ as in problem 2.