A Feynman-Kac Formula Implementation for the Linearized Poisson-Boltzmann (LPB) Equation

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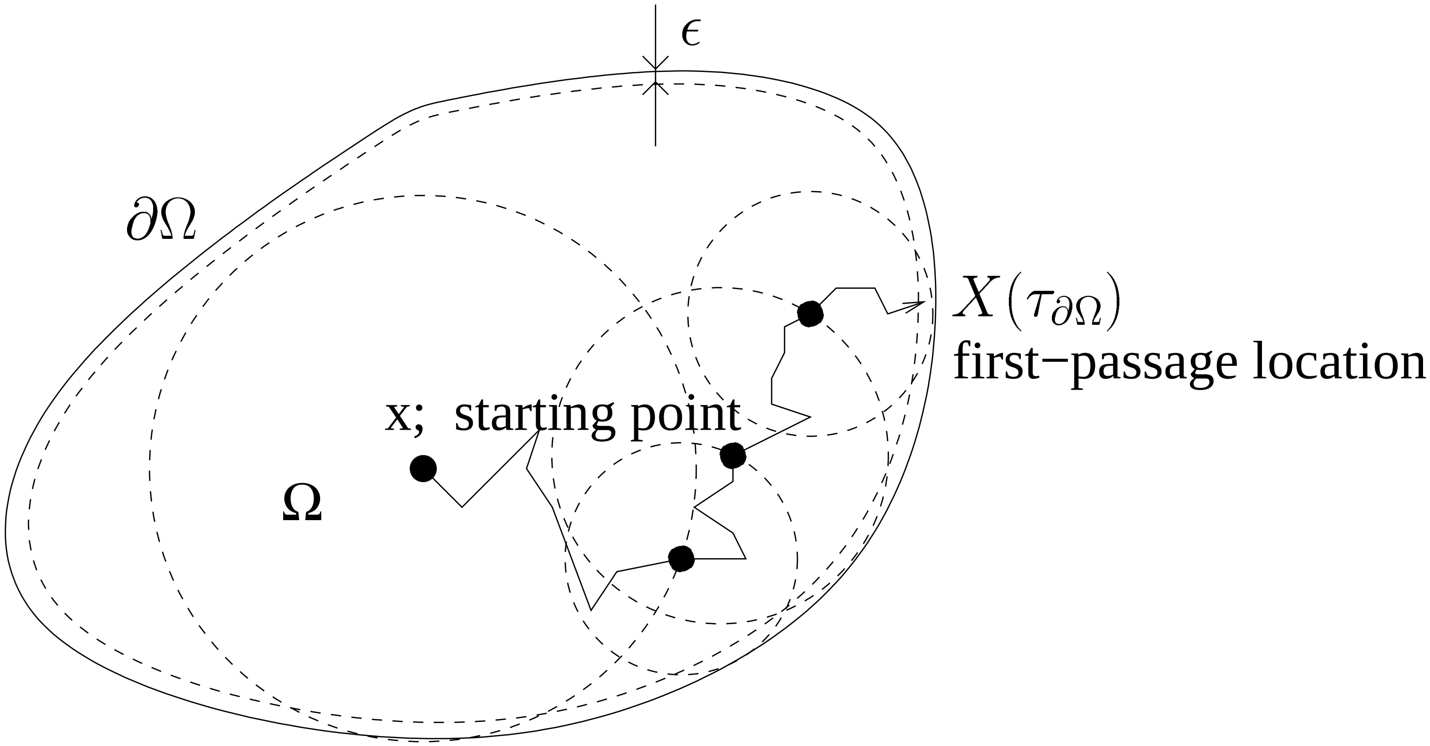
WOS for 2-D



ϵ
$\partial\Omega$
$X(\tau_{\partial\Omega})$
first−passage location
x; starting point
Ω

Dirichlet Problem for LPB

$$\nabla^2\psi(\mathbf{x}) = \kappa^2\psi(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \tag{1}$$

$$\psi(\mathbf{x}) = \psi_0(\mathbf{x}), \qquad \mathbf{x} \in \partial\Omega, \tag{2}$$

- Elepov-Mihailov solution:

$$u(\mathbf{x_0}) = \frac{1}{N}\sum_{i=1}^{N} Q_i^{n_i}\psi_0(X_{n_i}), \tag{3}$$

where

$$Q_i^0 = 1, \qquad Q_i^{n_i} = Q_i^{n_i-1}\frac{d_i^{n_i-1}\kappa}{\sinh(d_i^{n_i-1}\kappa)}, \qquad d_i^{n_i} = d(P_i^{n_i}). \tag{4}$$

Dirichlet Problem for LPB

- Elepov-Mihailov solution:
  - N: total number of diffusing random walkers
  - i refers to ith random walker
  - X_{n_i}: position where the ith random walker is absorbed in the ϵ-absorption layer after n_i WOS steps
  - $d_i^{n_i}$: radius of n_ith WOS of the ith random walker
    $\rightarrow$ survival probability of a random walker in a continuous and free diffusion region

$$p(d) = d\kappa / \sinh(d\kappa), \tag{5}$$

Dirichlet Problem for LPB

- Feynman-Kac representation of the solution:

$$u(\mathbf{x}) = E[\psi_0(X(\tau_{\partial\Omega}))\exp\{-\int_0^{\tau_{\partial\Omega}} \kappa^2 d\tau\}], \quad (6)$$

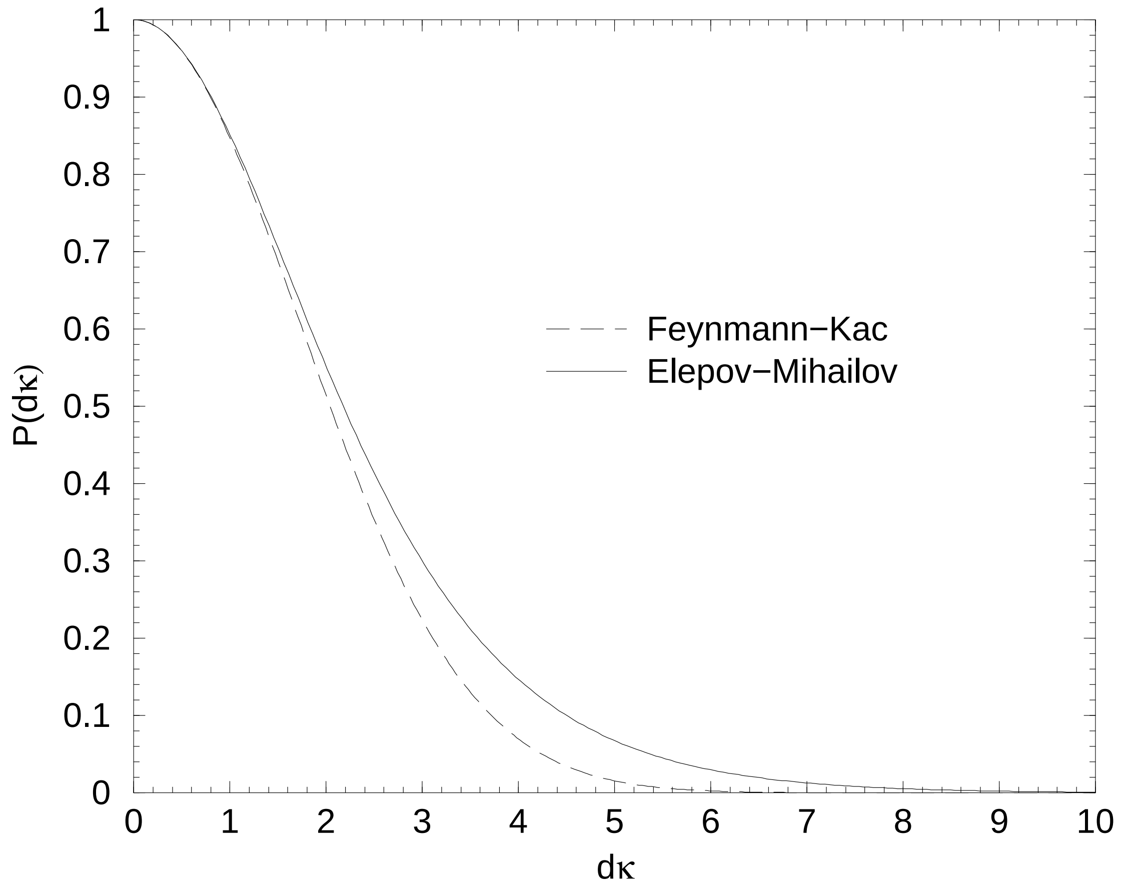
  – $\tau_{\partial\Omega} = \{\tau : X(\tau) \in \partial\Omega\}$: the first passage time

  – $X(\tau_{\partial\Omega})$: the first passage location on the boundary, $\partial\Omega$

  $\rightarrow$ survival probability of a random walker in a continuous and free diffusion region using the first moment of the first-passage time distribution

$$\exp(-\kappa^2 d^2/6), \quad (7)$$

Survival Probabilities



Equivalence of FK to EM

$$\int_0^\infty \frac{\partial P(t')}{\partial t'} \exp(-t'\kappa^2 d^2) dt' \tag{8}$$

$$= 2\sum_{n=1}^{\infty} (-1)^n (-n^2\pi^2) \int_0^\infty \exp[-(n^2\pi^2 + \kappa^2 d^2)t'] dt' \tag{9}$$

$$= -2\sum_{n=1}^{\infty} \frac{(-1)^n}{1 + \kappa^2 d^2/(n^2\pi^2)} \tag{10}$$

$$= \frac{\kappa d}{\sinh(\kappa d)}, \tag{11}$$

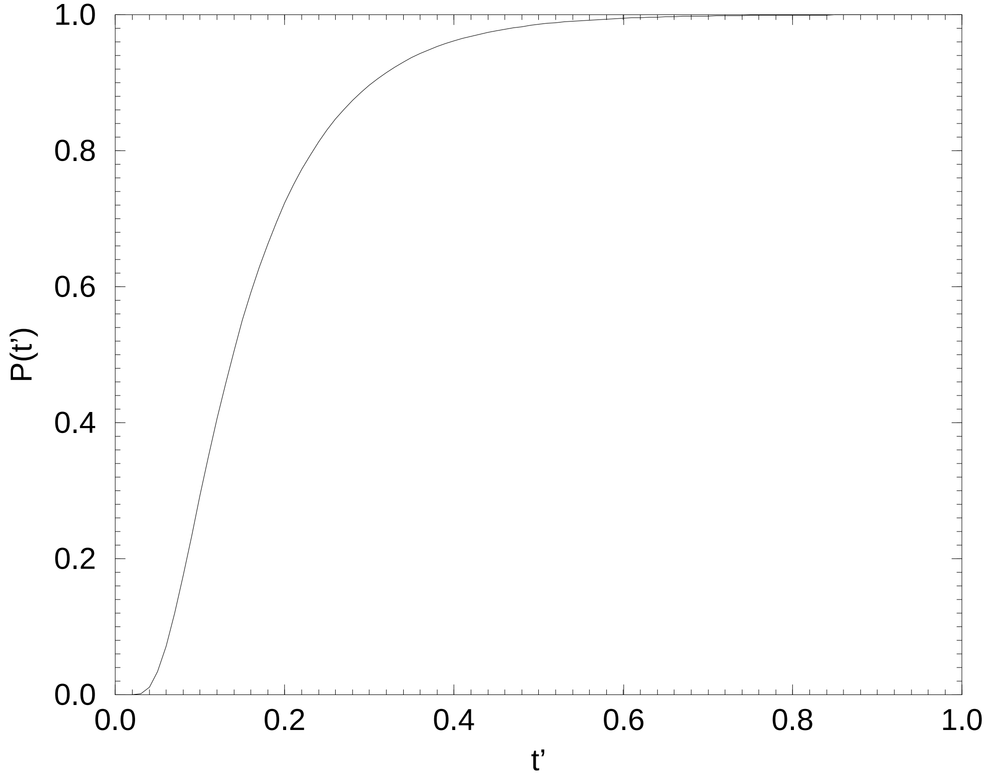
Equivalence of FK to EM

where the first passage time probability distribution, $P(t')$, is

$$P(t') = 1 + 2\sum_{n=1}^{\infty}(-1)^n \exp(-n^2\pi^2 t'). \qquad (12)$$

- t': $D\tau/d^2$
  - D: diffusion constant
  - τ: first passage time
  - r: radius of WOS

First-passage Time Probability Distribution



Feynman-Kac Implemetation for LPB

For each WOS step,

- Sampling t' using a random number in $(0, 1)$
- Corresponding survival probability, $\exp(-t' d^2 \kappa^2)$, is obtained
- Survival probability is compared with a random number in $(0, 1)$ and if the random number is greater than the survival probability, the random walker is removed at this WOS step.

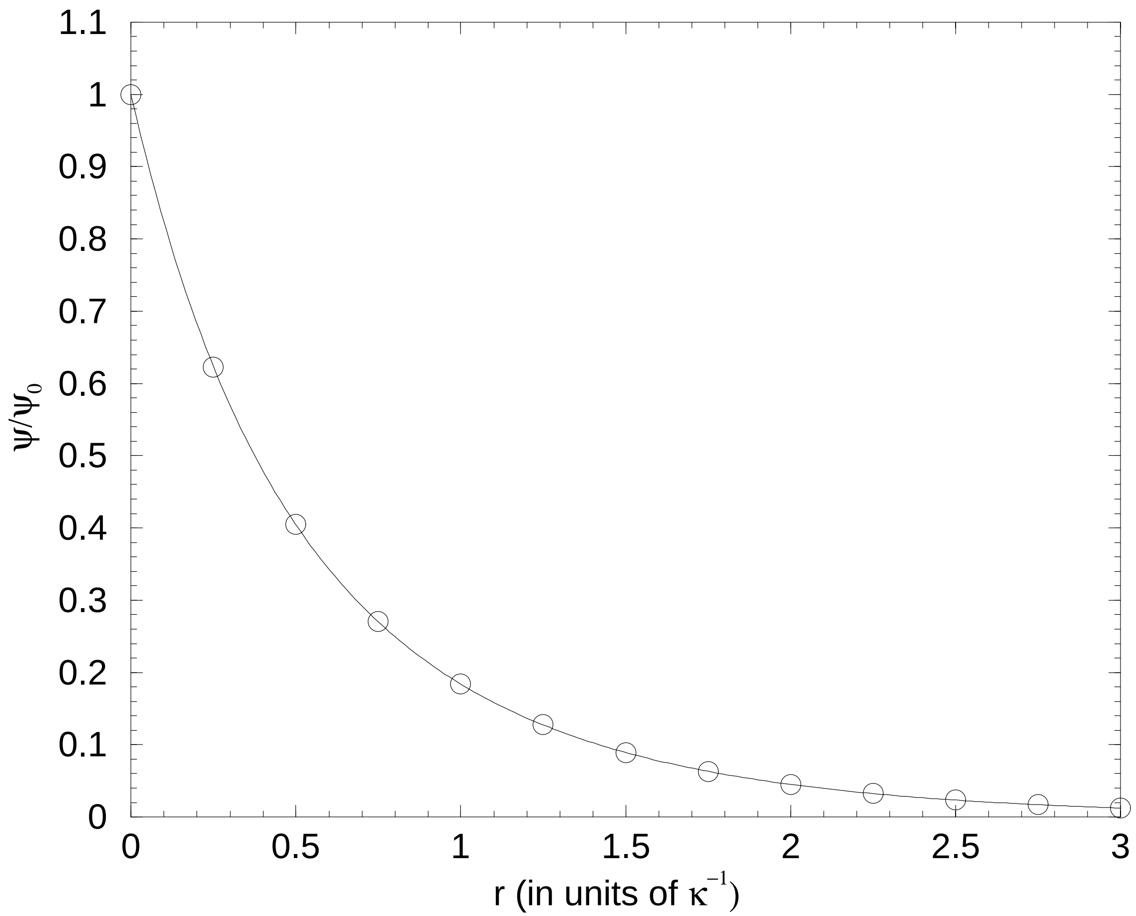
Dirichlet Problem for LPB

- An estimate for the solution at $\mathbf{x_0}$:

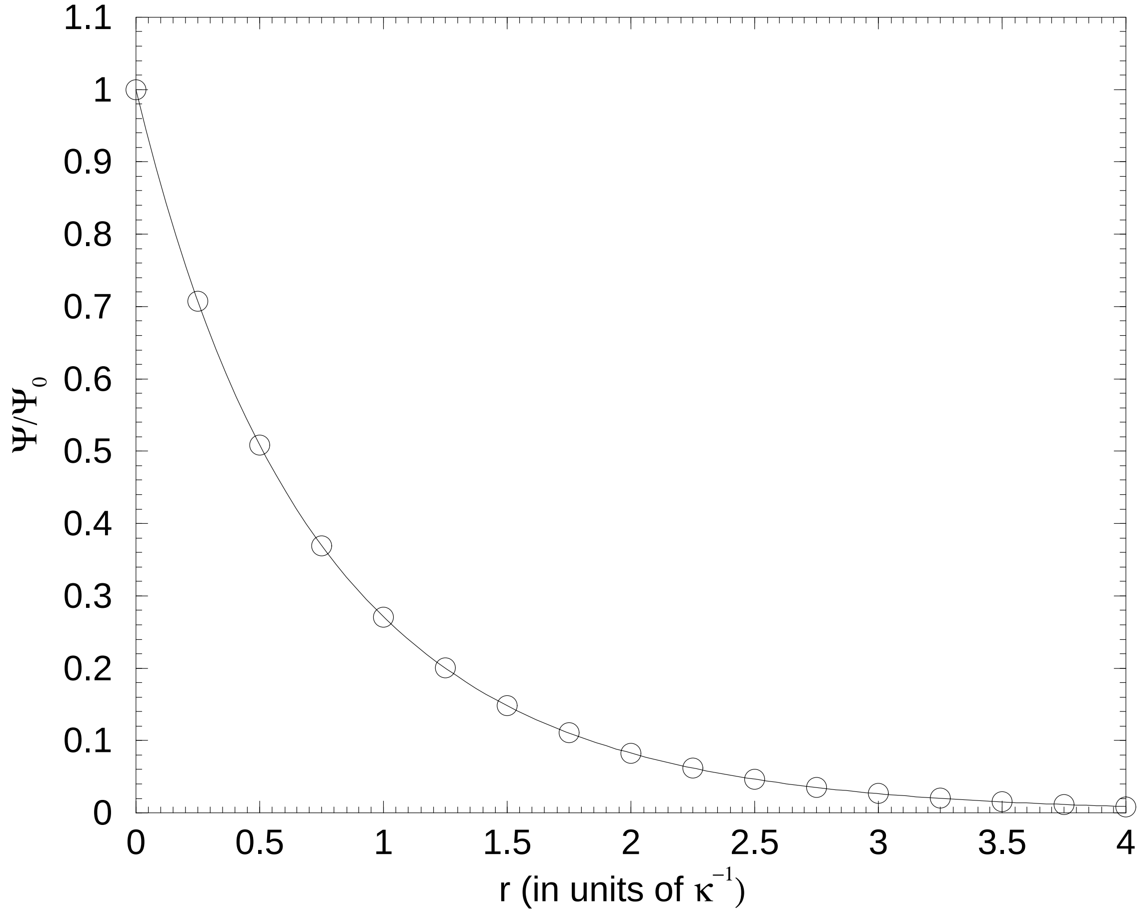
$$S_N = \frac{1}{N}\sum_{i=1}^{N_s}\psi_0(X_{n_i}) \tag{13}$$

  - N: number of trajectories
  - N_s: number of survived-and-absorbed random walkers
  - X_{n_i}: final position of the walker on the boundary when it is absorbed after n_i WOS steps

Sphere

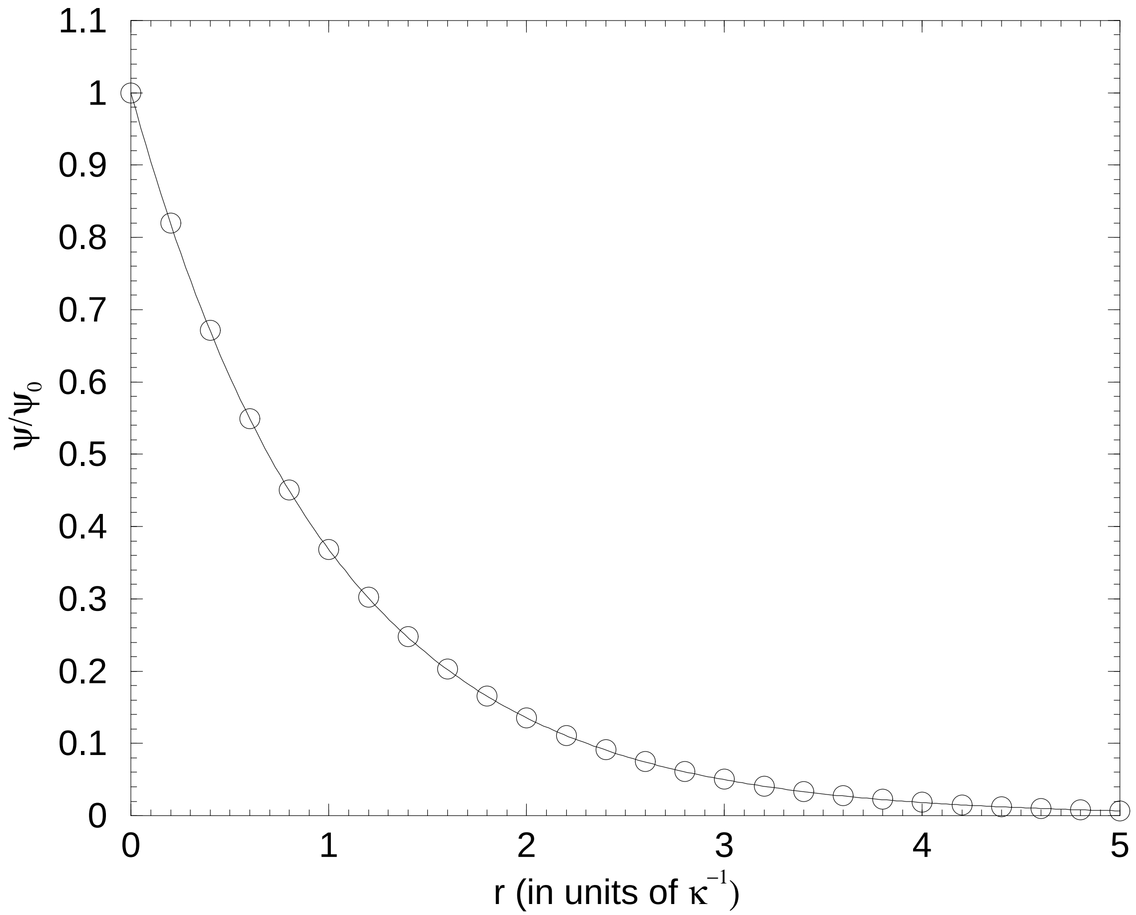


Cylinder

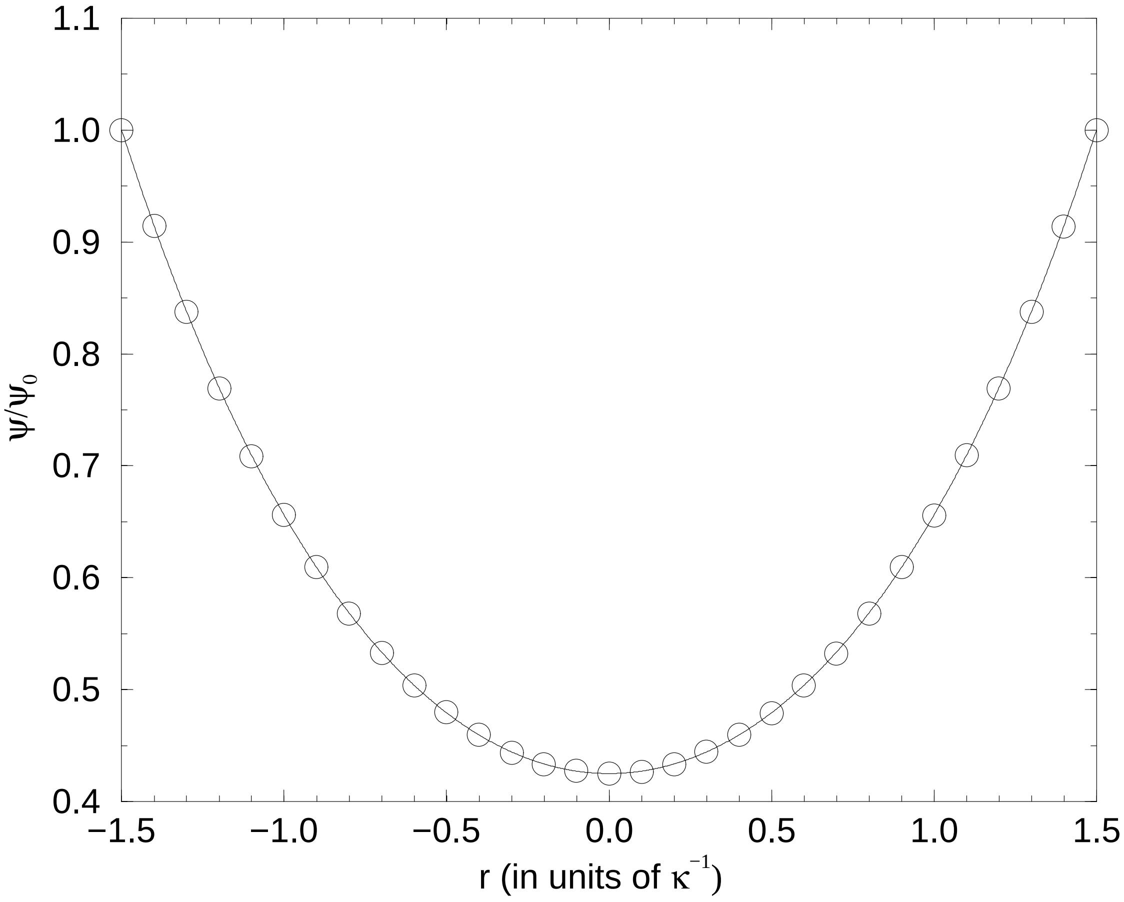


Ψ/Ψ0
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.5
1
1.5
2
2.5
3
3.5
4
r (in units of κ⁻¹)

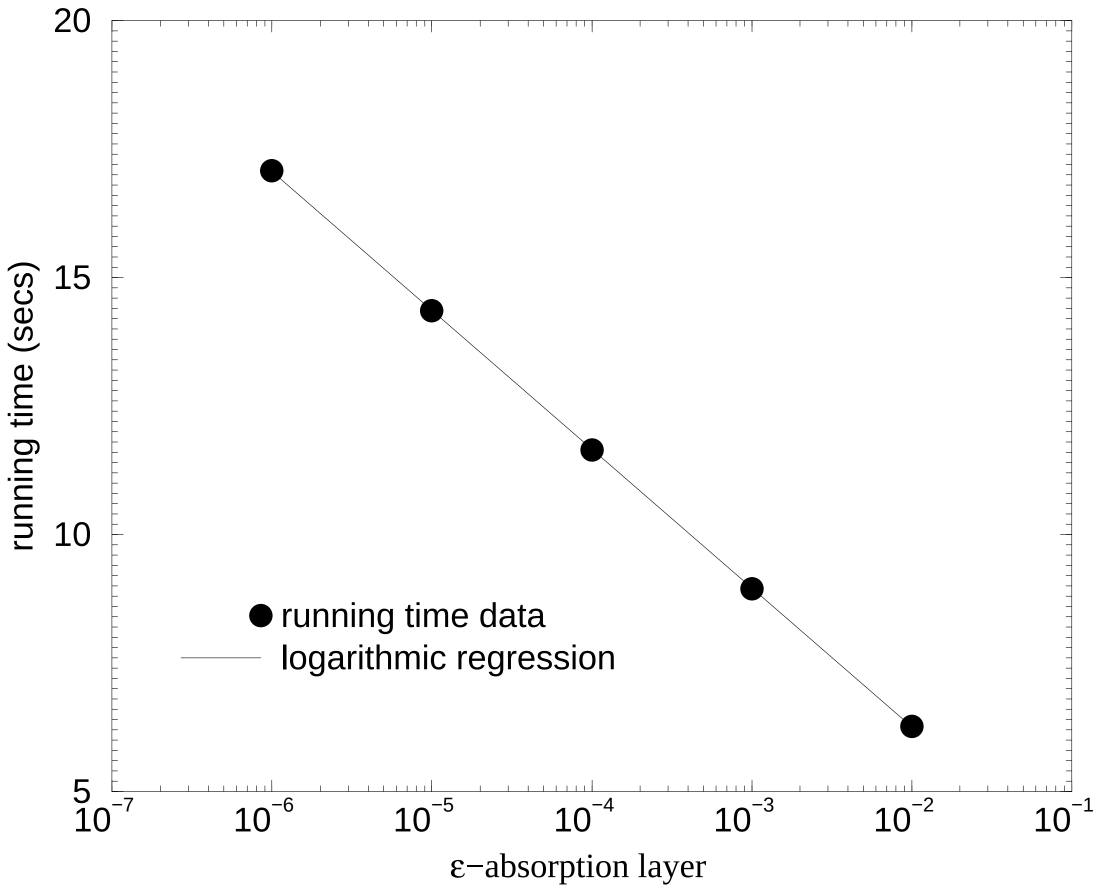
Plate



Parallel Plates



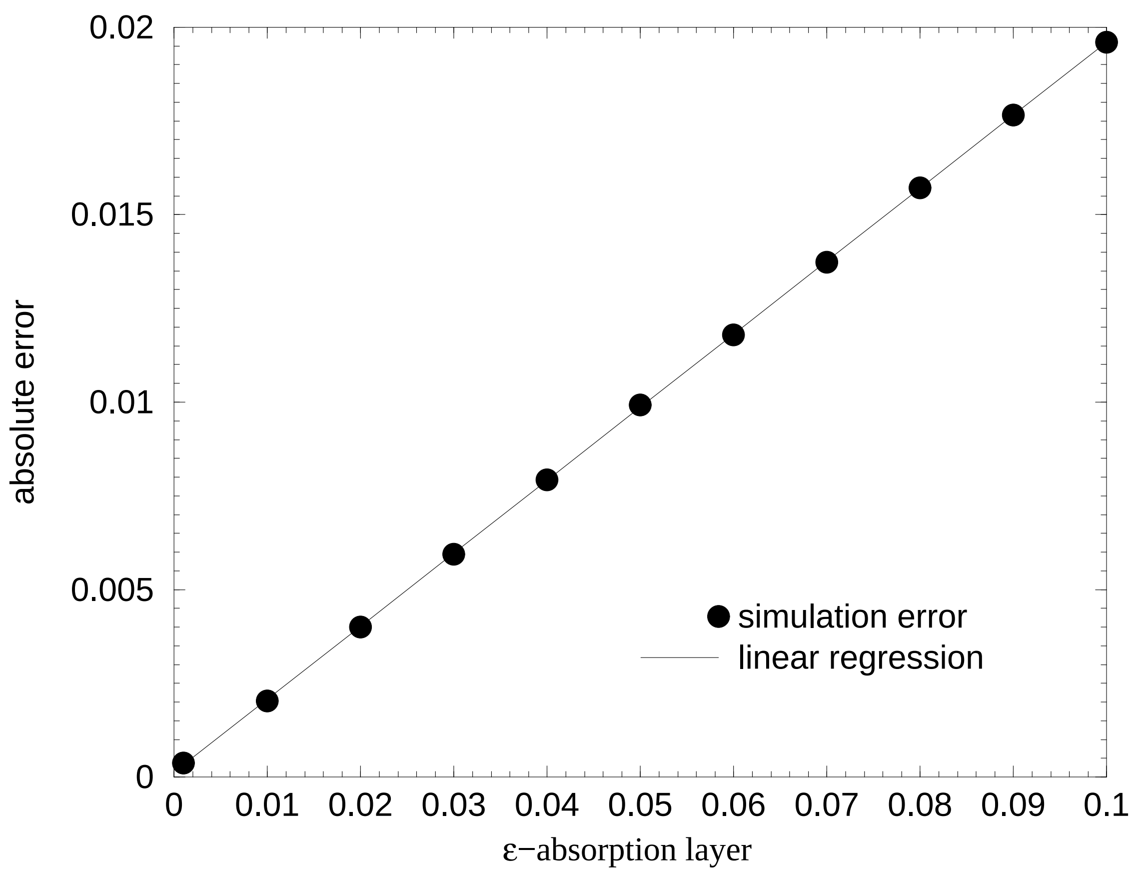
Runtime *w.r.t.* ϵ-absorption Layer



Errors

- Errors associated with the number of trajectories
  - can be reduced by increasing the number of trajectories
- Errors associated with the ϵ-absorption layer
  - It is possible to investigate empirically using enough number of trajectories

Errors from ϵ-absorption Layer



Future Work

- Solving $\Delta\psi(\mathbf{x}) - \kappa^2\psi(\mathbf{x}) = -g(\mathbf{x})$
- Extension to a method for the time-independent Schrödinger equation
- Quasirandom walks