Solution of Eigenvalue Problems for Multi-Scale Phenomena by Quantum Monte Carlo Methods

Peter Nightingale

Department of Physics, University of Rhode Island, Kingston RI 02881, USA

INTRODUCTION

- Particle in semi-infinite square well of depth -1 and width 1

  Unbinding transition: reduce mass; at a critical mass the last bound state acquires infinite range and disappears

- Dimensionless binding energy of ^{4}He dimer (Hurly-Moldover ϕ_{00} potential): -0.0002 (2 mK)

- Schloss Ringberg (1997) cluster meeting panel discussion:

  find the number of excited states of small He clusters

Problem: Approximate n energy eigenfunctions as linear combinations of n basis functions $\beta_1, \ldots, \beta_n$

$$\tilde{E} = \frac{\int \psi^*(R)\, \mathcal{H}\, \psi(R)\, dR}{\int \psi^*(R)\psi(R)\, dR}$$

$$\frac{\delta \tilde{E}}{\delta \psi(R)} \propto (\mathcal{H} - \tilde{E})\psi(R)$$

Stationary linear combination: gradient perpendicular to all basis functions

$$\langle \beta_i | (\mathcal{H} - \tilde{E}) \sum_j d_j |\beta_j\rangle \;=\; 0$$

$n \times n$ eigenvalue equation:

$$\mathbf{N}^{-1}\mathbf{H}\mathbf{d}^{(k)} = \tilde{E}_k \mathbf{d}^{(k)}$$

with

$$N_{ij} = \langle \beta_i | \beta_j \rangle$$
$$H_{ij} = \langle \beta_i | \mathcal{H} | \beta_j \rangle$$

Yield:

exact		approximate
$\psi^{(k)}(R)$	$\approx$	$\tilde{\psi}^{(k)}(R) = \sum_i \beta_i(R)\, d_i^{(k)}$
E_k	$\lesssim$	$\tilde{E}_k$

Optimization of linear prams

$\mathbf{N}^{-1}\mathbf{H}$ from a small MC sample; zero-variance principle: exact eigenvectors in span$(\beta_1, \ldots, \beta_n)$ no statistical errors Numerical instability: $\mathbf{N}$ often nearly singular

Optimization of non-linear prams

Basis functions β_i depend on non-linear parameters. Optimize by minimization of

$$\frac{\langle \tilde{\psi}^{(k)} | (\mathcal{H} - \tilde{E}_k)^2 | \tilde{\psi}^{(k)} \rangle}{\langle \tilde{\psi}^{(k)} | \tilde{\psi}^{(k)} \rangle}$$

[C. J. Umrigar et al., Phys. Rev. Lett. **60,** 1719 (1988)].

Optimizations use small, fixed MC sample of 10^4 configs, SCALAPACK SVD, enhanced Levenbergh-Marquardt. (22 node Beowulf cluster)

Reduction of variational bias

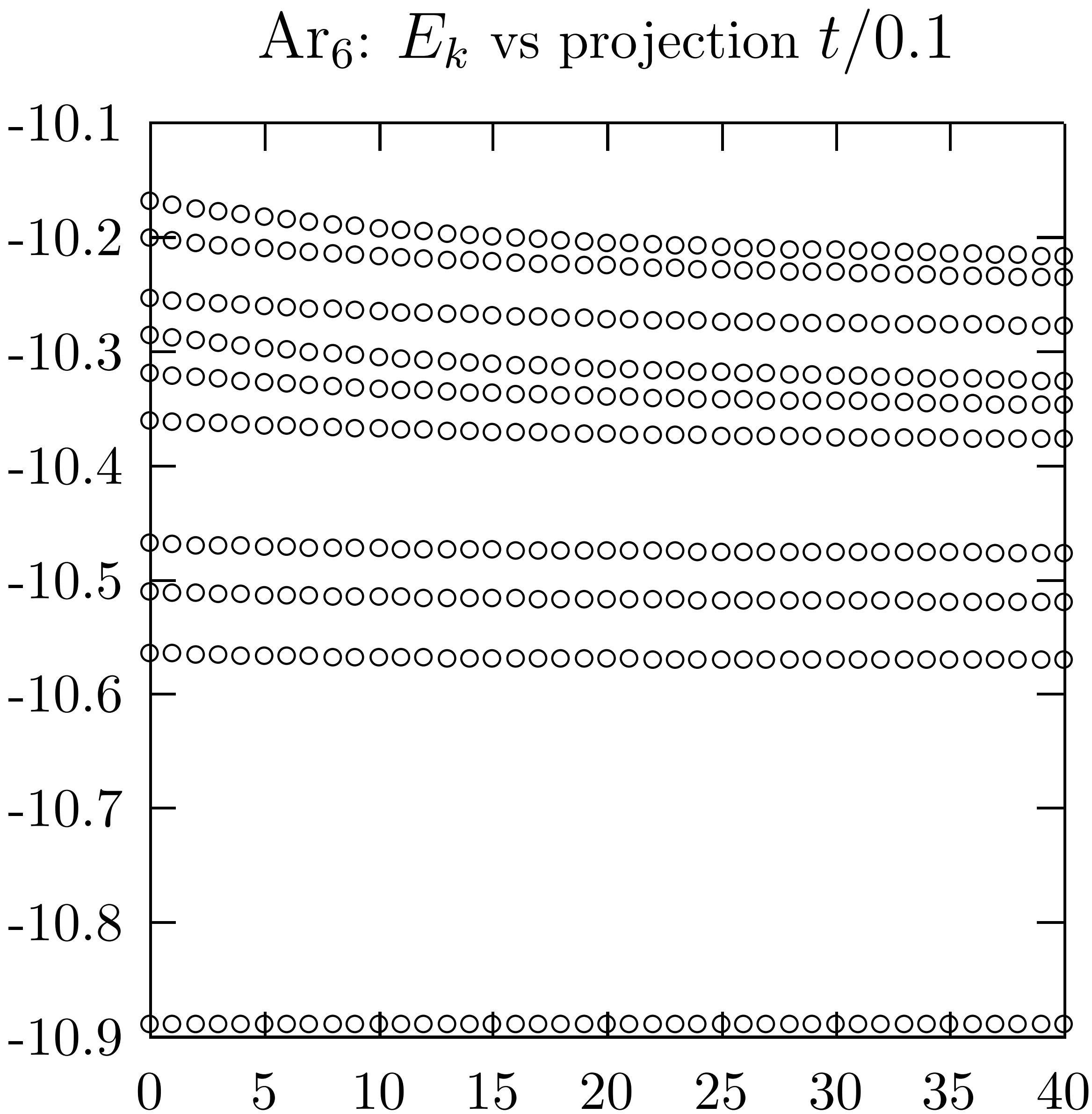
Diffusion MC to obtain

$$|\tilde{\psi}^{(k)}\rangle \to |\tilde{\psi}^{(k)}\rangle(t) \equiv \exp(-t\mathcal{H})|\tilde{\psi}^{(k)}\rangle$$

[D.M. Ceperley and B. Bernu, J. Chem. Phys. **89**, 6316 ('88)]

Pure DMC with large samples

Samples are generated with an optimized guiding function: maximize overlap with excited states; minimize fluctuations of re-weighting factors



Ar$_6$: E_k vs projection $t/0.1$
-10.1
-10.2
-10.3
-10.4
-10.5
-10.6
-10.7
-10.8
-10.9
0
5
10
15
20
25
30
35
40

FIG. 1. Ne: N=6 lowest 5 states

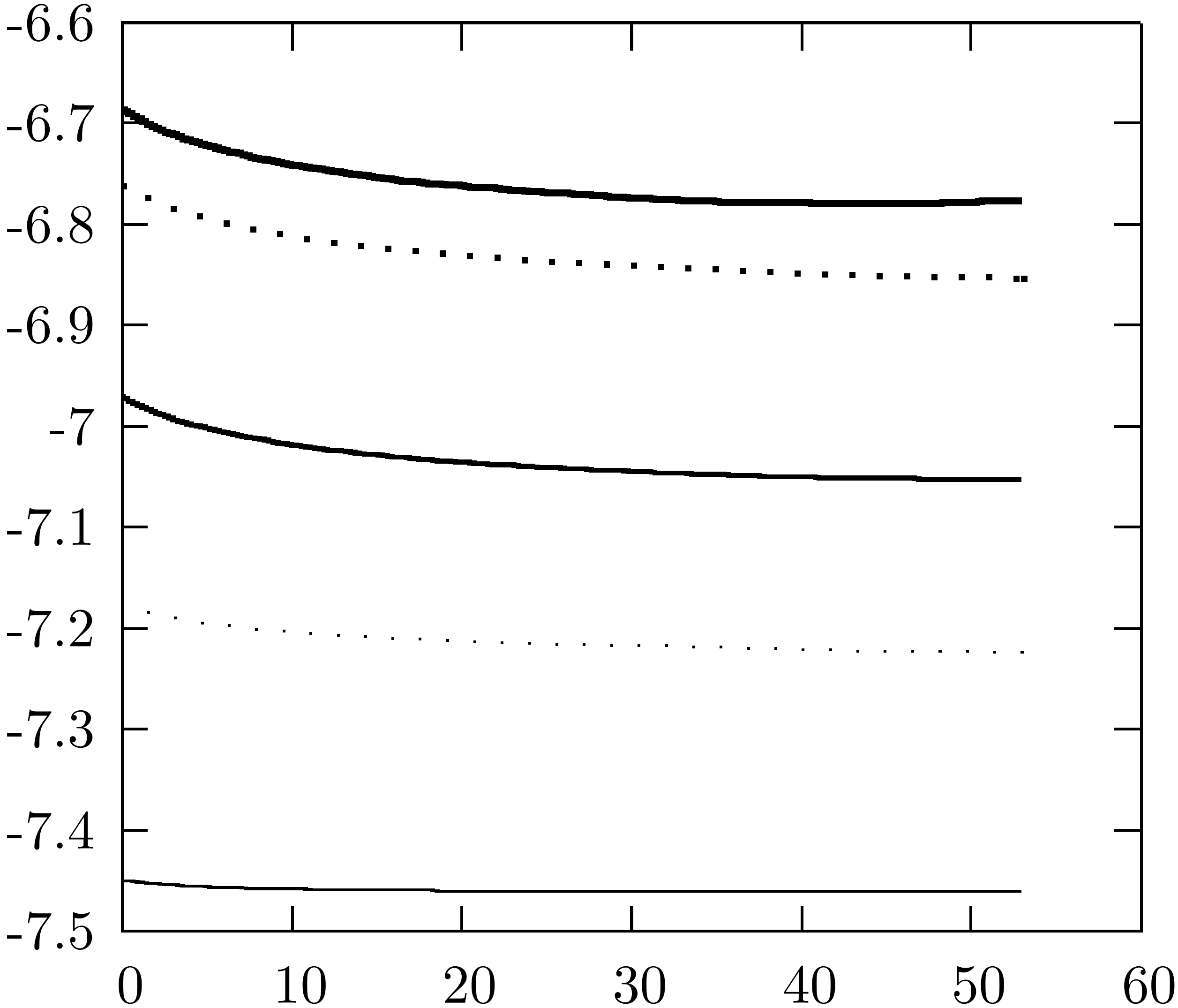


FIG. 2. N=4 VMC energies

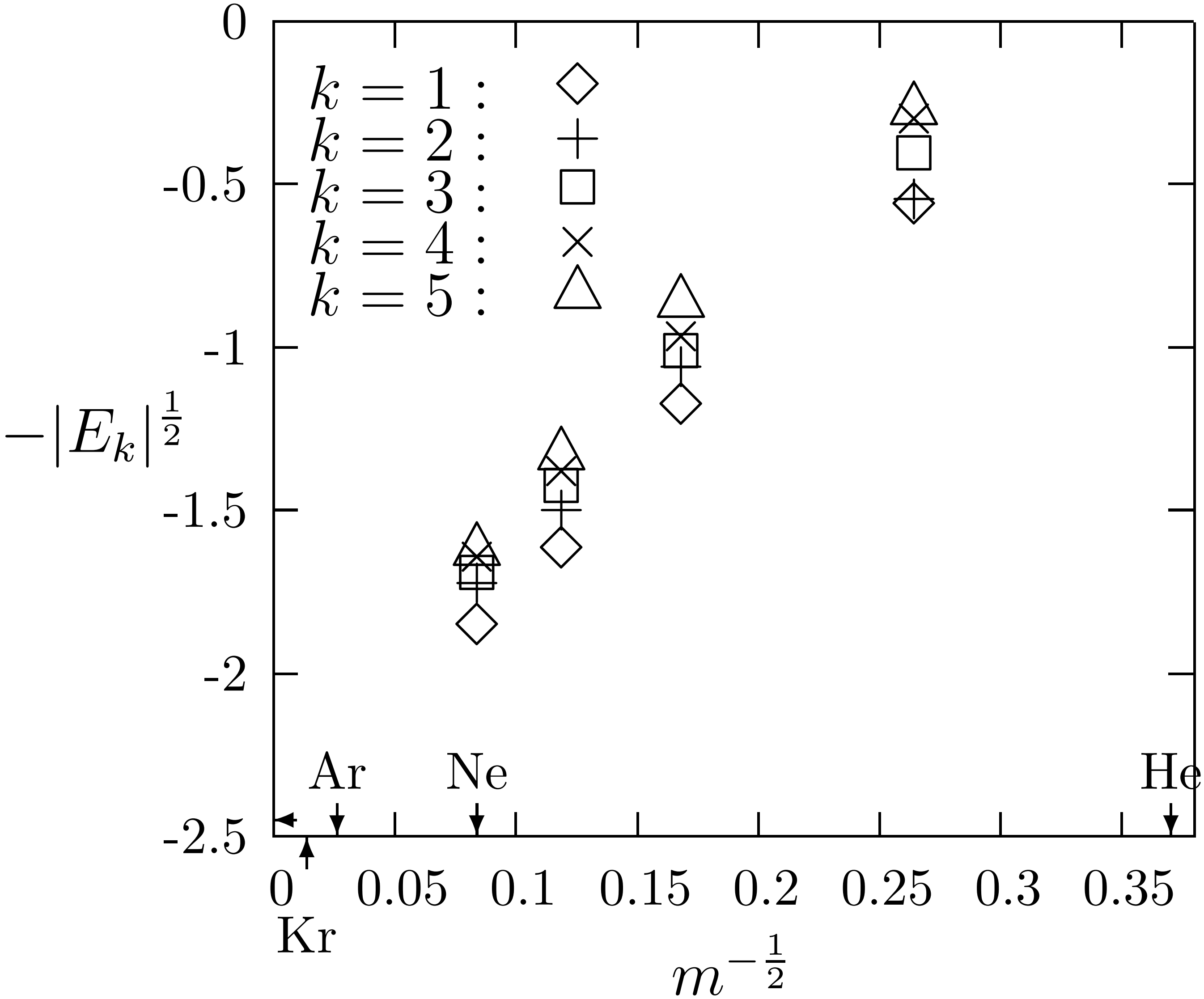


FIG. 3. N=4 DMC energies at $t = 10 \times 0.1$