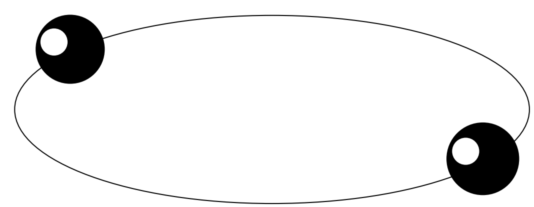
Quantum Rings

Comparison of ED and VMC. . . and perhaps some more



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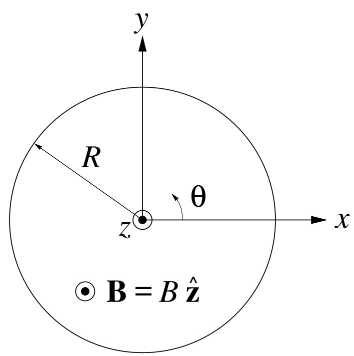
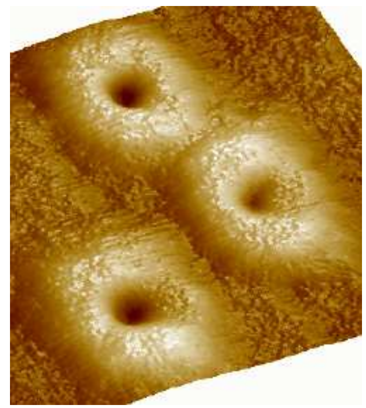
Overview

- Introduction.
- Basics.
- Computational methods.
- ED accuracy.
- Groundstate configurations.
- Results:
  - Ground state energy.
  - Angular momentum distribution.
  - Pair distribution function.
- Fractional Periodicity.

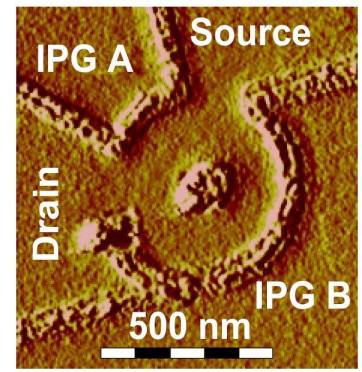
Introduction

- Semiconductor quantum rings :





A. Lorke et al. PRL **84** *2223 (2000).*



U. F. Keyser, PhD Thesis.

- In a magnetic field, a persistent current flows.
- Spectrum periodic in magnetic flux.

Basics

$$\mathcal{H} = \sum_i \mathcal{H}_0(\theta_i) + \sum_{i<j} V(\theta_{ij}), \quad \mathcal{H}_0 \left|\phi_l\right\rangle = \epsilon_l \left|\phi_l\right\rangle,$$

where $l = 0, \pm 1, \pm 2, \ldots$ and

$$\epsilon_l = \frac{\hbar^2 l^2}{2m^* R^2} \quad \text{and} \quad \langle \mathbf{r} | \phi_l \rangle = \frac{e^{-il\theta}}{\sqrt{2\pi R}}$$

Coulomb interaction:

$$V(\theta_{ij}) = \frac{V_C}{\sqrt{r_{ij}^2 + \tilde{\mu}^2}}$$

Here $V_C = 0.1, 1, 10$, corresponding to $R = 2 \ldots 200$ nm.

Parameter $\tilde{\mu}$ gives a width.

Computational Methods

Exact Diagonalization (ED):

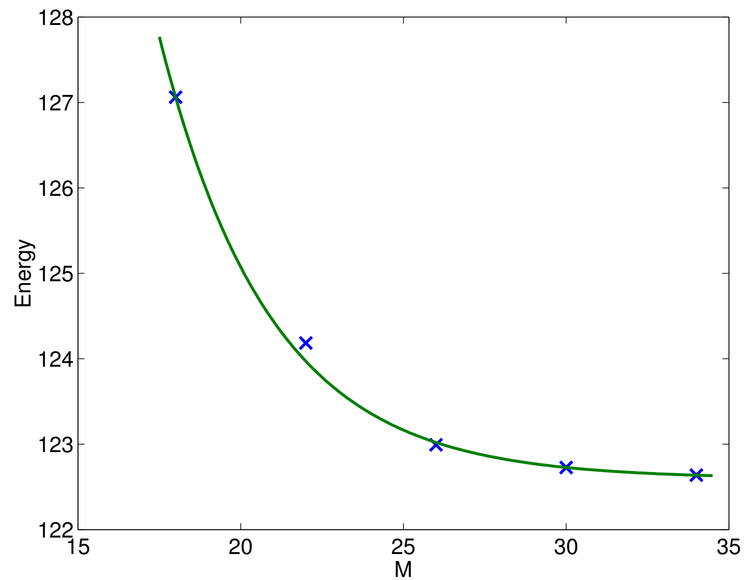
- Expand $|\Psi\rangle$ in a Slater basis and solve matrix Schrödinger eq.
- In principle exact, but in practice basis must be finite.
- Very heavy in computations so number of e^{-}'s restricted to $\lesssim 6$.

Variational Quantum Monte Carlo (VMC):

- Can handle large systems.
- Although an approximation has proved to be very accurate in many cases.

ED Convergence

Worst-case Scenario:



- $N = 6, V_C = 10, M_{\max} = 34$.
- #Slater dets is

$$\binom{M}{N} = 1344904$$

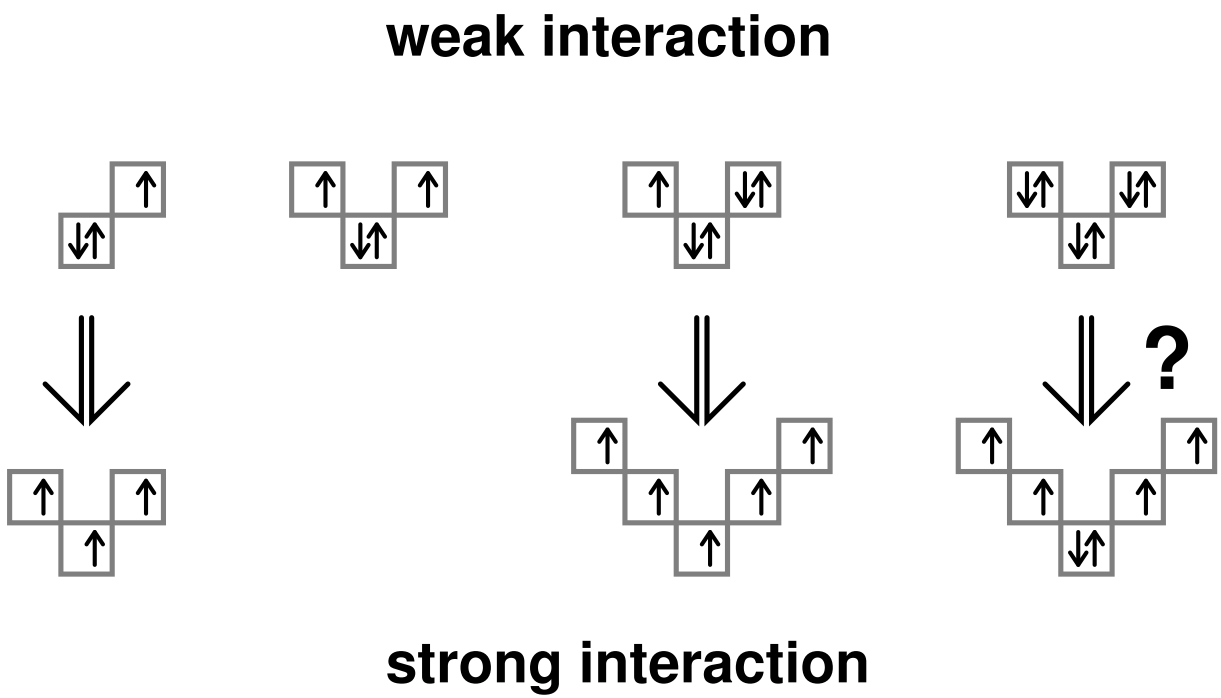
but size of $\mathcal{H} \simeq 16000^2$.

Fit: $E(M) = E_0 + \alpha e^{-\beta M} \Rightarrow \boxed{E_0 \simeq 122.60}$.

$E_{ED} = 122.638 \quad E_{VMC} = 122.866 \pm .004 \quad E_{HF} = 152.32$

$\rightarrow$ ED has sufficient accuracy to test VMC quality.

Configurations



- Weak V_C: Compact arrangement minimizes kinetic nrg.
- Strong V_C: Closed shells of one spin type, finite spin polarization.

Ground State Energy

% of correlation energy captured by VMC:

$$E_c = \frac{E_{HF} - E_{VMC}}{E_{HF} - E_{ED}}$$

V_C	$N = 2$	$N = 3$	$N = 4$	$N = 5$	$N = 6$
0.1	0.987(2)	0.888(6)	0.966(9)	0.900(4)	0.937(7)
1	0.9960(4)	0.992(2)	0.9838(5)	0.9505(5)	0.9652(6)
10	0.99991(1)	0.9982(2)	0.9975(1)	0.9900(1)	0.9922(1)

VMC more accurate for high (low) V_C (N).

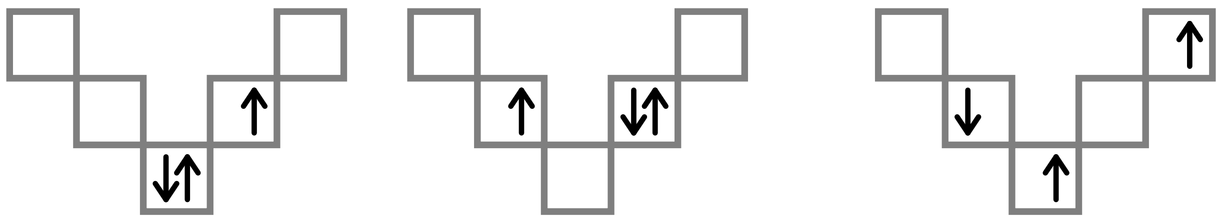
VMC performs worst in open-shell cases. Why?

Open-shell Case

VMC wavefunction expanded in ED basis and weights of most important configurations compared to ED results.

Example:

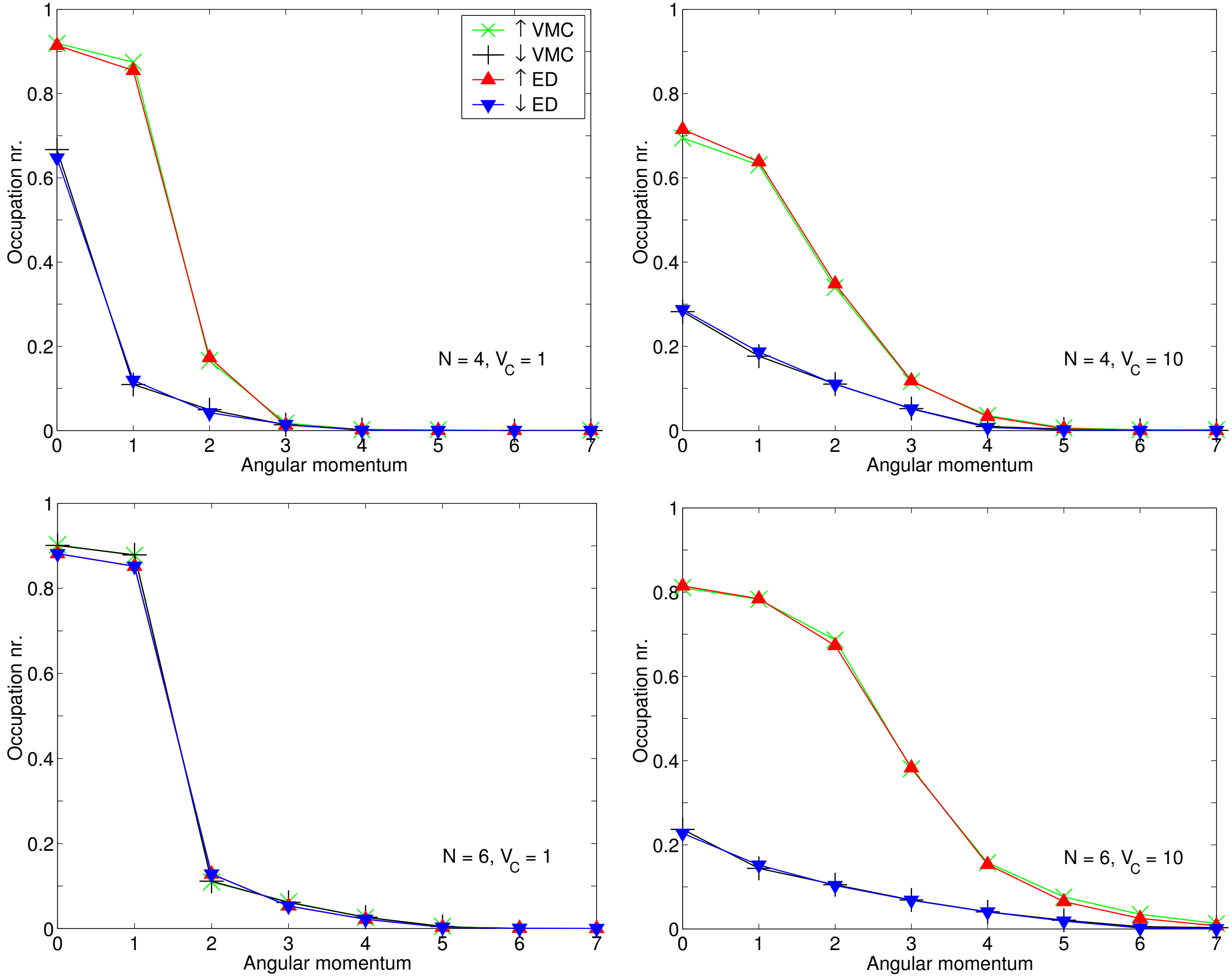
N = 3, V = 0.1



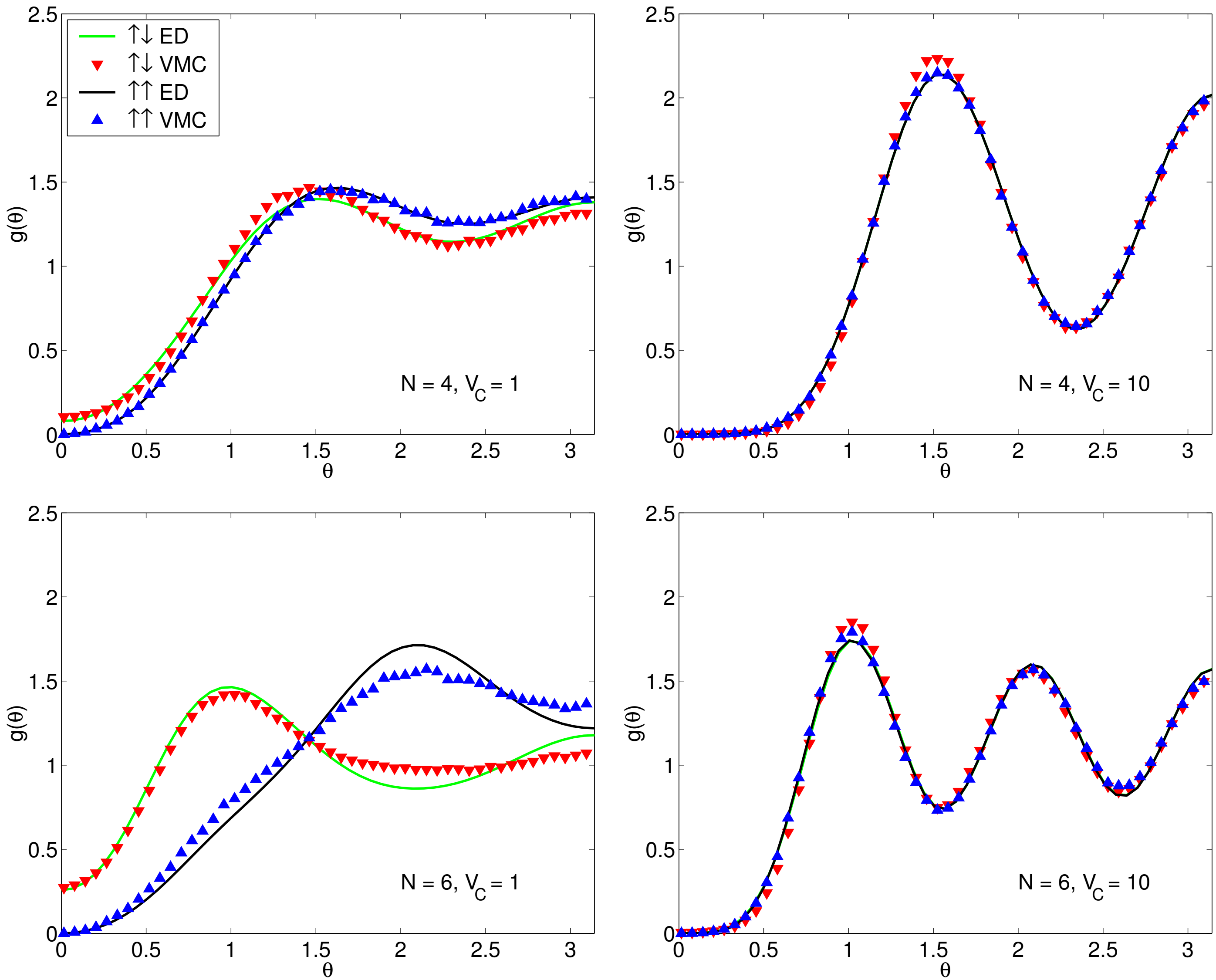
ED:	97.1%	1.9%	0.47%
VMC:	97.9%	0.84%	0.84%

$L = 1$ $\Delta(l_{\uparrow} - l_{\downarrow}) = \pm 2$

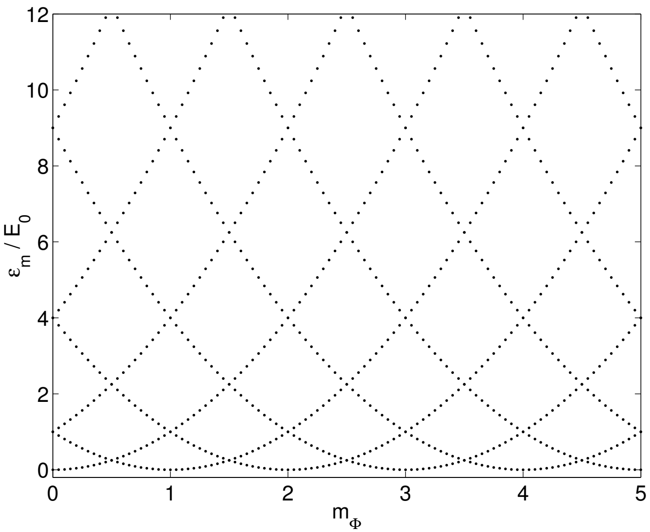
Occupation Distribution



Pair Distribution Function

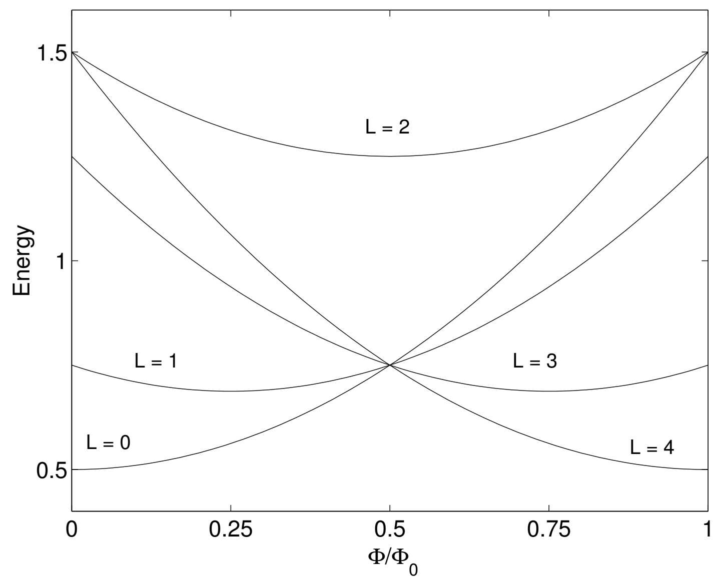


Fractional Periodicity



Magnetic field $\rightarrow$
s-p spectrum Φ_0-periodic.

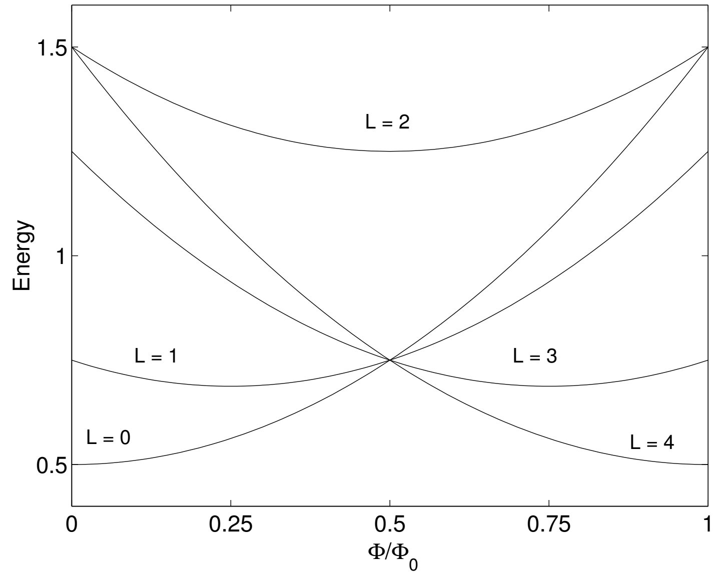
Fractional Periodicity



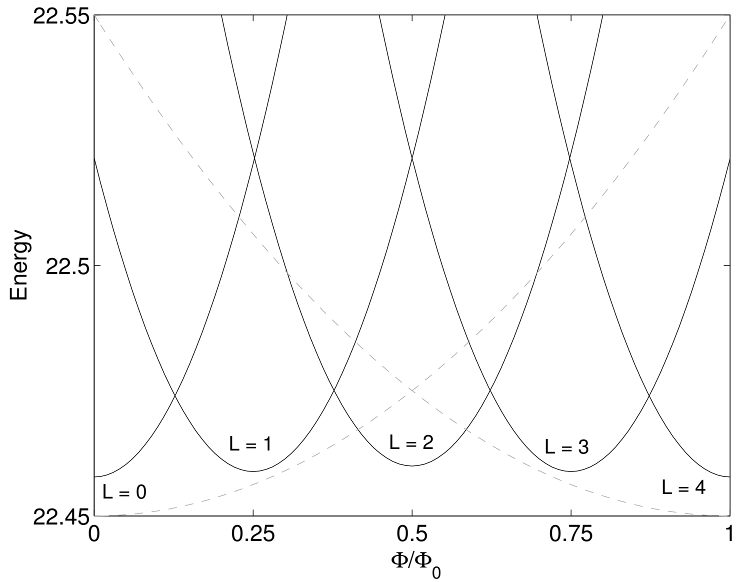
$N = 4, S_z = 1, V_C = 0$

Period $\Phi_0 = h/e$

Fractional Periodicity

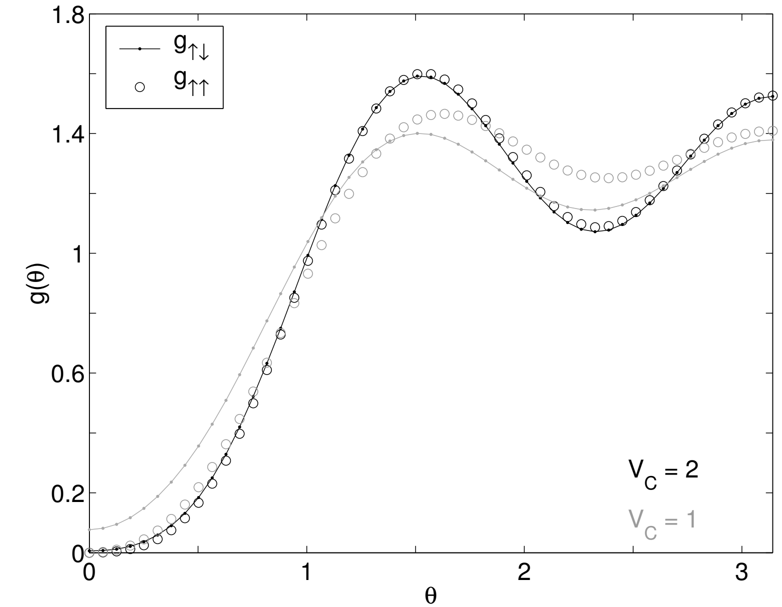


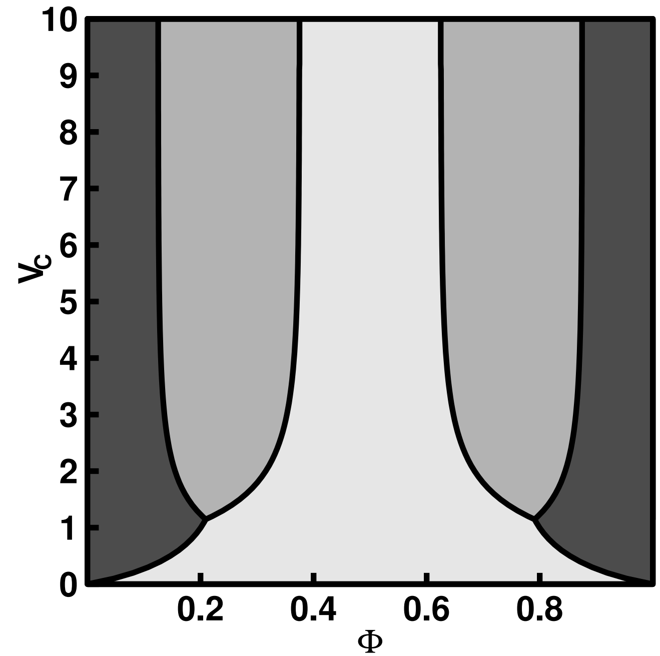
$N = 4, S_z = 1, V_C = 0$
Period $\Phi_0 = h/e$

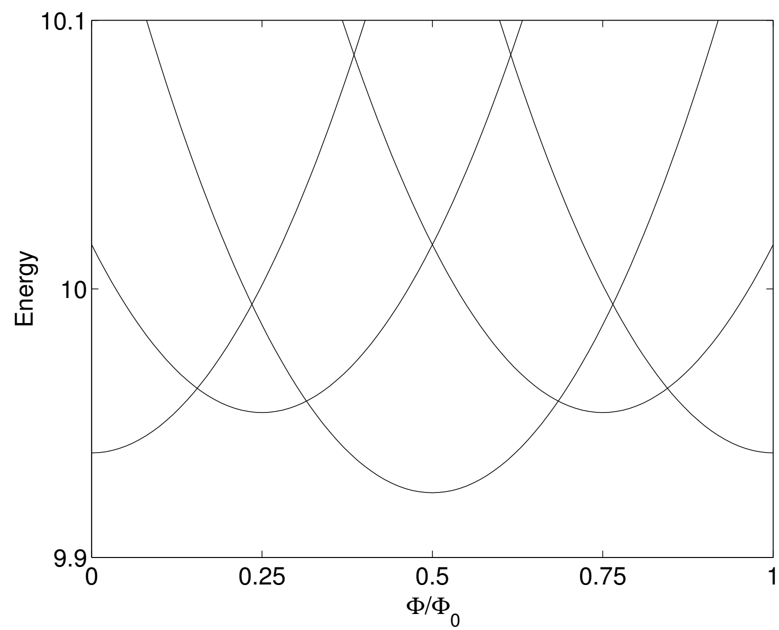


$N = 4, S_z = 1, V_C = 5$
Period $\Phi_0/4$

Fractional Periodicity







$N = 4, S_z = 1.$