Application of SSE on different quantum many-body systems

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量子磁性与多体计算培训班
CSRC，2024

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Reference

1. "Quantum Monte Carlo simulation method for spin systems" Anders W. Sandvik and Juhani Kurkijärvi, Phys. Rev. B 43, 5950 (1991)---original paper of SSE
2. "Stochastic series expansion method with operator-loop update" Anders W. Sandvik, Phys. Rev. B 59, R14157(R) (1999)---operator-loop with link table
3. "Quantum Monte Carlo with directed loops" Olav F. Syljuåsen and Anders W. Sandvik Phys. Rev. E 66, 046701 (2002) ---Direct loop
4. "Directed loop updates for quantum lattice models" Olav F. Syljuåsen, Phys. Rev. E 67, 046701 (2003) ---Direct loop
5. "A generalization of Handscomb's quantum Monte Carlo scheme-application to the 1D Hubbard model" Anders W. Sandvik, J. Phys A: Math. Gen. 25 (1992) 3667-3682.---SSE measurement
6. "Generalized directed loop method for quantum Monte Carlo simulations" Fabien Alet, Stefan Wessel, and Matthias Troyer, Phys. Rev. E 71, 036706 (2005)---relation between SSE and worm algorithm
7. "Path-integral computation of superfluid densities"E. L. Pollock and D. M. Ceperley, Phys. Rev. B 36, 8343 (1987)---superfluid density measurement

Outline

- Review of SSE
- Quantum magnetism
- Optical lattice
- Rydberg array

Review of SSE

Stochastic Series Expansion

$$Z = \langle \exp(-\beta H) \rangle$$

$$= \sum_{\alpha} \sum_{n=0}^{+\infty} \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle$$

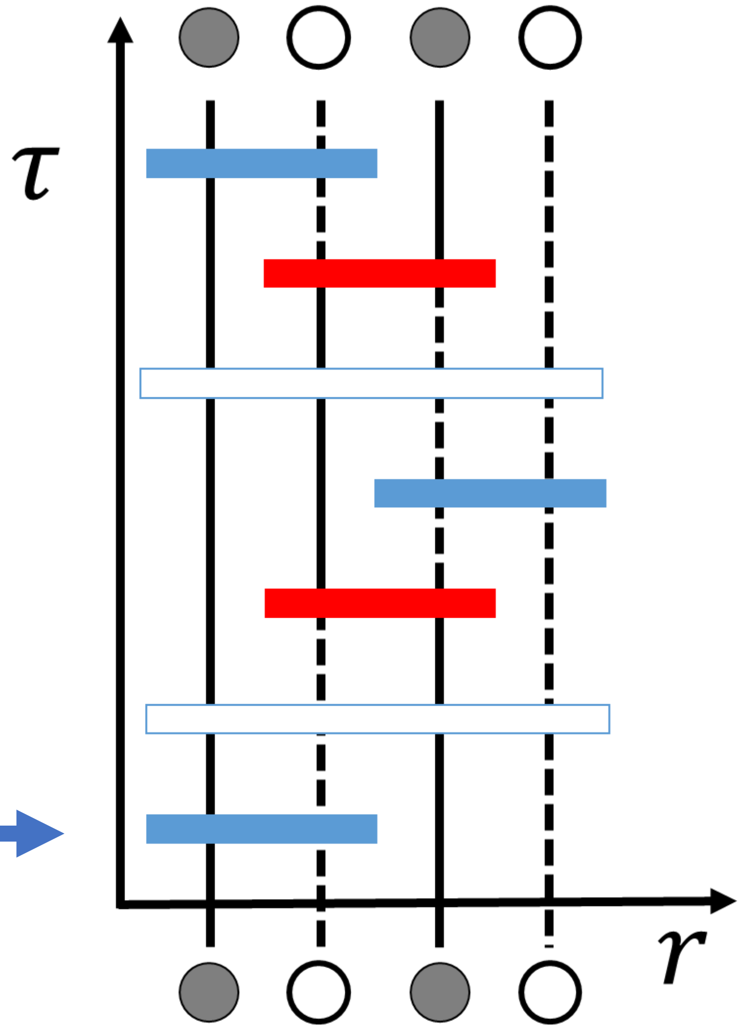
$$H = -\sum_{\{a_i, b_i\}} H_{\{a_i, b_i\}}$$

$$= \sum_{\alpha} \sum_{n=0}^{+\infty} \sum_{S_n} \frac{\beta^n}{n!} \left\langle \alpha \left| \prod_{i=1}^{n} H_{\{a_i, b_i\}} \right| \alpha \right\rangle$$

Insert $H_{0,0}$

$$\overset{M \to +\infty}{=} \sum_{\alpha} \sum_{S_n} \frac{\beta^n (M-n)!}{M!} \left\langle \alpha \left| \prod_{i=1}^{M} H_{\{a_i, b_i\}} \right| \alpha \right\rangle$$

Diagram mapping



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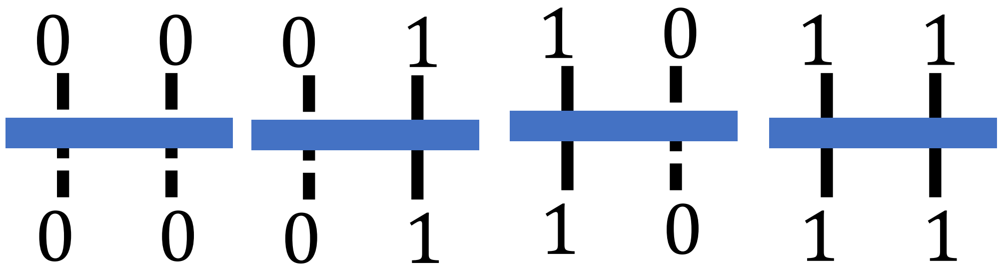
Stochastic Series Expansion

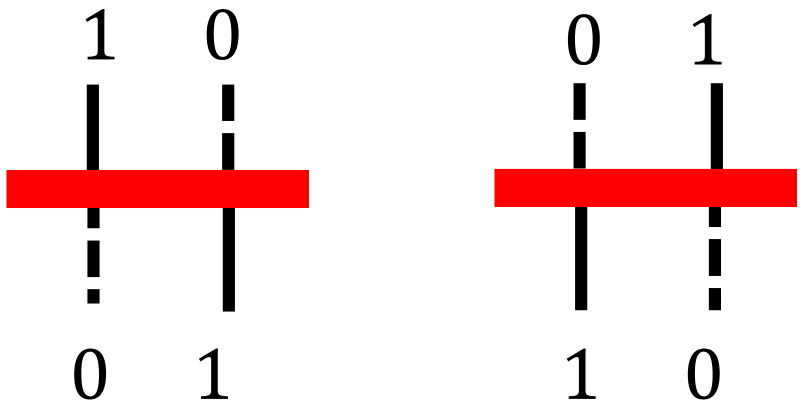
$$H = -t\sum_{\langle i,j\rangle}(S_i^+S_j^- + h.c.) + V\sum_{\langle i,j\rangle} S_i^Z S_j^Z$$

1: ↑   0: ↓

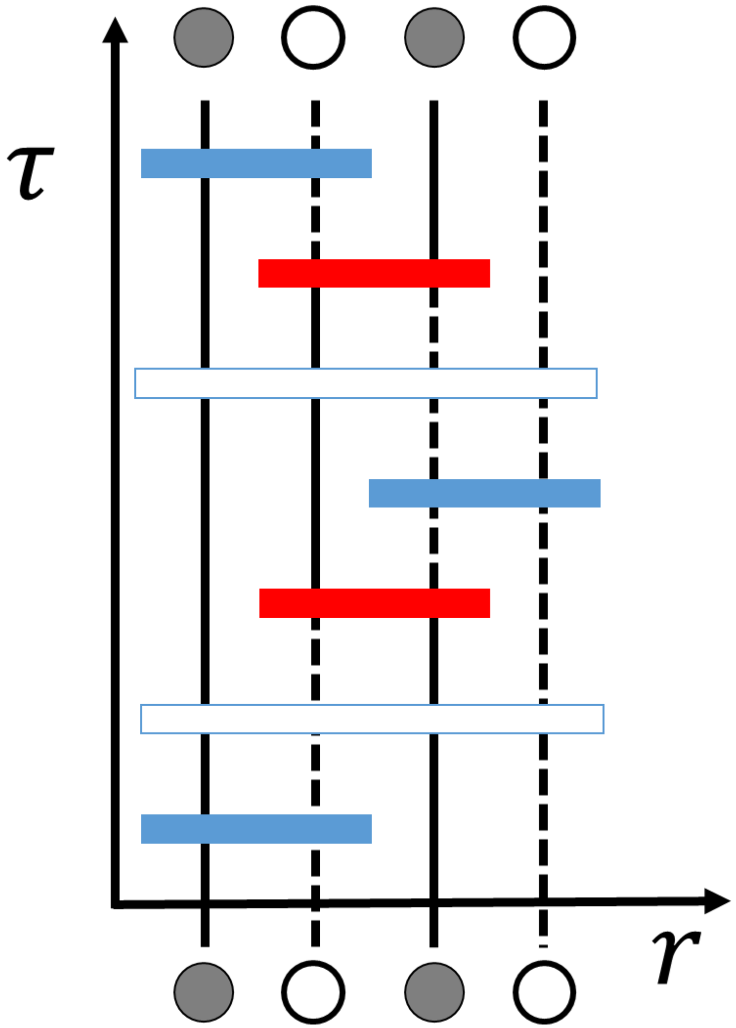
Diagonal Operators



Off-Diagonal Operators



Unit Operators (Zero-operator)



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Structure of the program

1. Initialization of RNG;
2. Initialization of Lattice;
3. Initialization of vertex weight;
4. Initialization of transfer matrix and probability;
5. Initialization of configuration and operator list;
6. #======Thermalization loop=====
7. for i=1:istp
8.   diagonal update();
9.   loop update();
10.   adjust truncation dimension M;
11. end
12. #======Measurement loop=====
13. for i=1:mstp
14.   diagonal update();
15.   loop update();
16.   measure();
17. end
18. writing data

Initialization of RNG

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```
#---------Begining of part1 RNG---------
#Initialization of the 64-bits LXM LCG
seed=Int64(2024);  #The seed of RNG LCG64
#The parameter of the LCG64
const lcg_a=Int64(2862933555777941757)
const lcg_c=Int64(3037000493)
#The precision of the LCG64
const lcg_eps=-0.5/(Int64(2)^63)
#The function of the LCG64
function lcg(x0)
    x0=lcg_a*x0+lcg_c;    #The equation of the iteration
    return x0;            #X_n -> X_{n+1}
end
function rndm()
    global seed=lcg(seed);
    return seed*lcg_eps+0.5
end
#----------End of part1 RNG-------------
#  ****************************************************
```

Chin. Phys. B 33, 037509 (2024)

COMPUTATIONAL PROGRAMS FOR PHYSICS

Analysis of pseudo-random number generators in QMC-SSE method

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(Received 13 November 2023; revised manuscript received 9 January 2024; accepted manuscript online 15 January 2024)

In the quantum Monte Carlo (QMC) method, the pseudo-random number generator (PRNG) plays a crucial role in determining the computation time. However, the hidden structure of the PRNG may lead to serious issues such as the breakdown of the Markov process. Here, we systematically analyze the performance of different PRNGs on the widely used QMC method known as the stochastic series expansion (SSE) algorithm. To quantitatively compare them, we introduce a quantity called QMC efficiency that can effectively reflect the efficiency of the algorithms. After testing several representative observables of the Heisenberg model in one and two dimensions, we recommend the linear congruential generator as the best choice of PRNG. Our work not only helps improve the performance of the SSE method but also sheds light on the other Markov-chain-based numerical algorithms.

LCG:

$$x_n = \mathrm{Mod}(a x_{n-1} + c, p)$$

Seed: x_0

Initialization of lattice

One dimensional chain:

```
#   ************************************************************
#----------Begining of part2 lattice-----
# The parameter of the lattice
ns=10::Int64; #Number of the sites or the system length
nb=ns;        #Number of bond is same as the number of sites
#The information of bond with periodical boundary condition
bond=zeros(Int,2,nb);
bond[1,:]=1:ns;bond[2,:]=[2:ns;1];
conf=zeros(Int64,ns);
for i=1:ns
    conf[i]=min(floor(Int64,rndm()*2.),1);
end
#storing the value of the spin 0 for spin down and 1 for spin up
#-----------End of part2 lattice----------
```

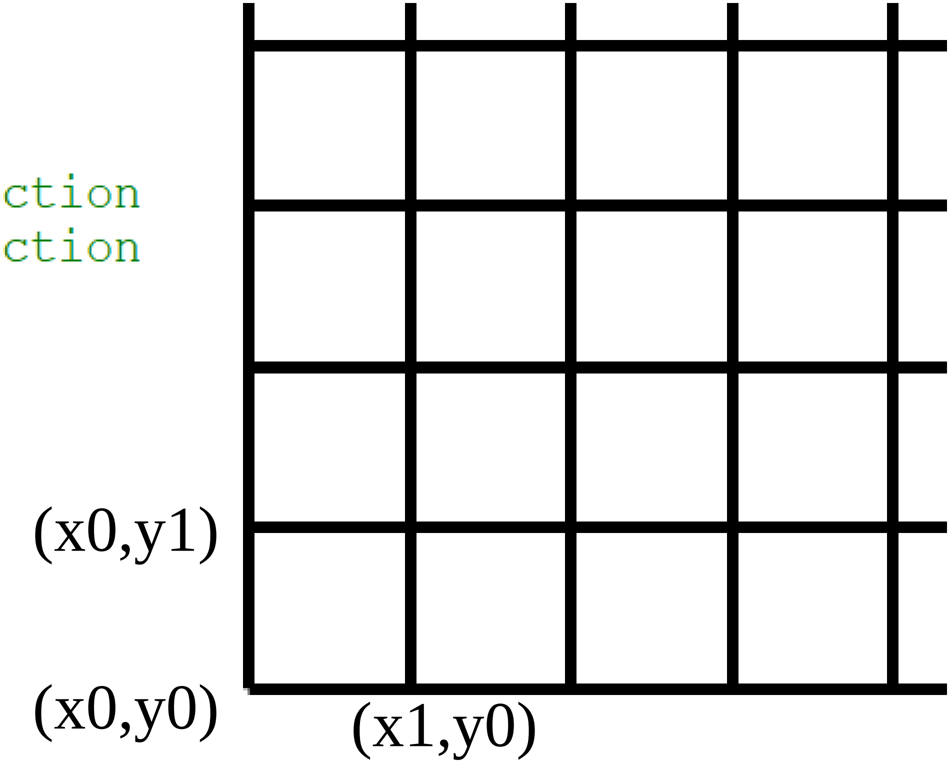
2D?

Initialization of lattice

Square Lattice:

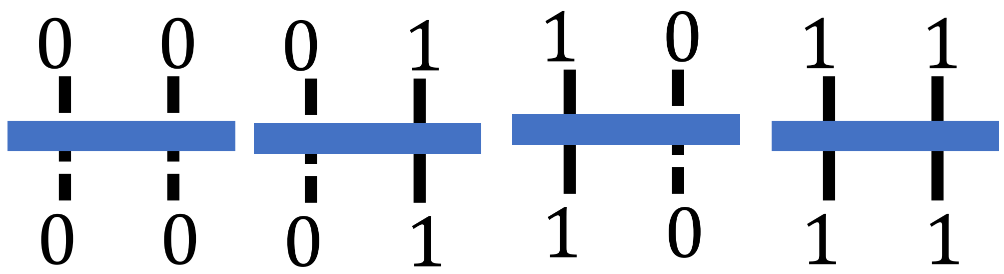
```
# The parameter of the lattice
nx=10::Int64 #system size in x
ny=10::Int64 #system size in y
ns=nx*ny::Int64; #Number of the sites
nb=2*ns;  #the number of bond is twice larger than the number of sites
#The information of bond with periodical boundary condition
bond=zeros(Int,2,nb);
is=0::Int64 #counting sites
for y0=1:ny
    for x0=1:nx
        is=is+1; #counting bond
        x1=x0%nx+1; #Next in x direction
        y1=y0%ny+1; #Next in y direction
        #Bond in x direction
        bond[1,is]=x0+(y0-1)*nx;
        bond[2,is]=x1+(y0-1)*nx;
        is=is+1;
        #Bond in y direction
        bond[1,is]=x0+(y0-1)*nx;
        bond[2,is]=x0+(y1-1)*nx;
    end
end
```

triangular?

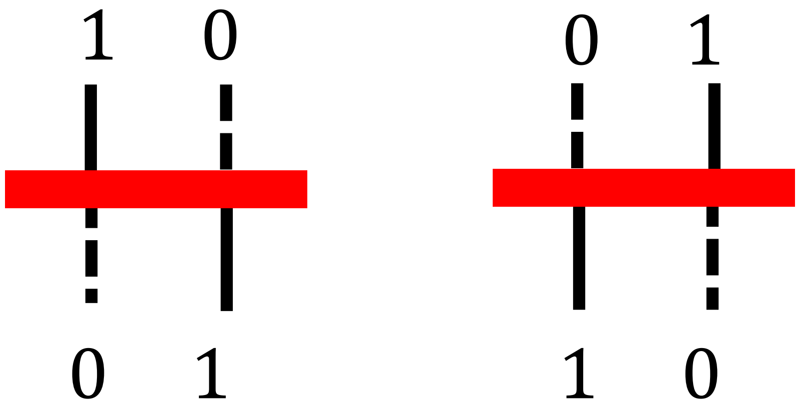


Initialization of vertex

Diagonal Operators



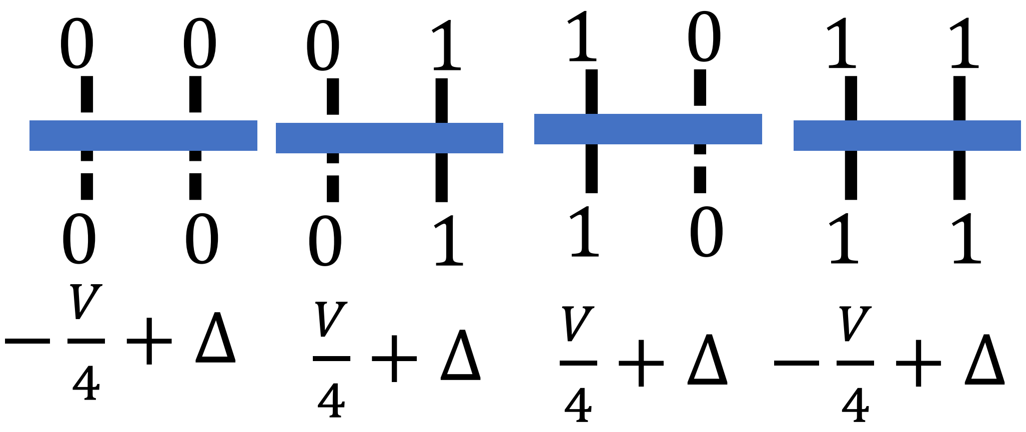
Off-Diagonal Operators



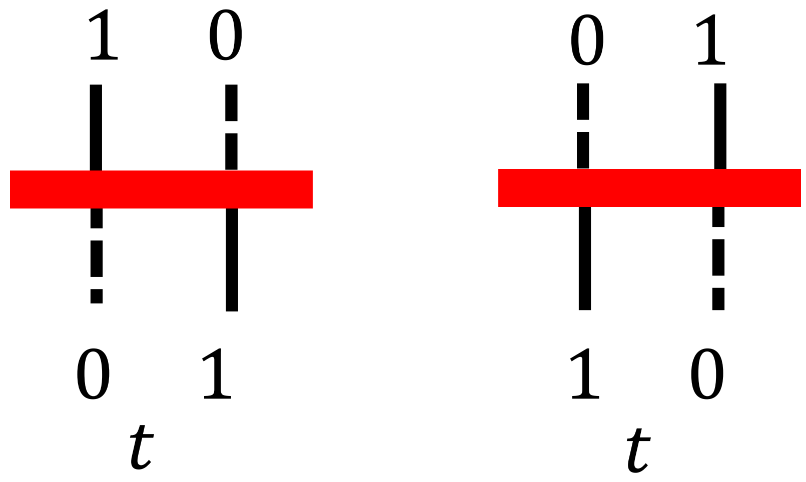

```
#-----------Begining of part3 vertex and weight--
#The parameter of the physical system
t=0.5::Float64;    #The off-diagonal interaction
V=1.::Float64;    #The diagonal interaction
beta=10.0::Float64;  #The inverse temperature
#--------Initialization of vertex------
#The configuration of vertexes
vtx=zeros(Int,6,4);
#diagonal operator
vtx[1,:]=[0 0 0 0];vtx[2,:]=[0 1 0 1];
vtx[3,:]=[1 0 1 0];vtx[4,:]=[1 1 1 1];
#off-diagonal operator
vtx[5,:]=[0 1 1 0];vtx[6,:]=[1 0 0 1];
#The reverse process with help of binary
#representation
vtx_rev=zeros(Int,4,4);
#diagonal operator
vtx_rev[1,1]=1;vtx_rev[2,2]=2;
vtx_rev[3,3]=3;vtx_rev[4,4]=4;
#off-diagonal operator
vtx_rev[2,3]=5;vtx_rev[3,2]=6;
```

Initialization of weight

Diagonal Operators



Off-Diagonal Operators



$$H=-t\sum_{\langle i,j\rangle}(S_i^+S_j^-+h.c.)+V\sum_{\langle i,j\rangle}S_i^ZS_j^Z$$

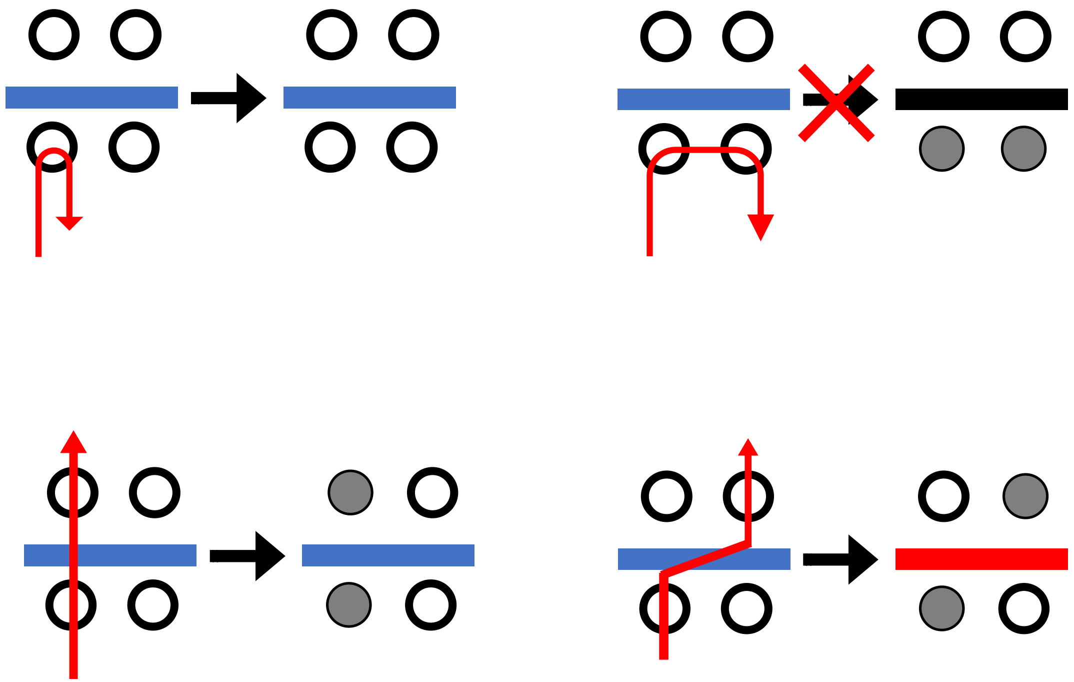
$$-B\sum_i S_i^Z\ ?$$

```
# Initialization of the weight of each operator
weight=zeros(6);
energy_shift=V/4+.5;
# Diagonal operator
weight[1]=-V/4;weight[2]=V/4;
weight[3]=V/4;weight[4]=-V/4;
weight[1:4]=weight[1:4].+energy_shift;
# off-diagonal operator
weight[5:6].=t;
#--------End of part3 vertex and weight---------
```

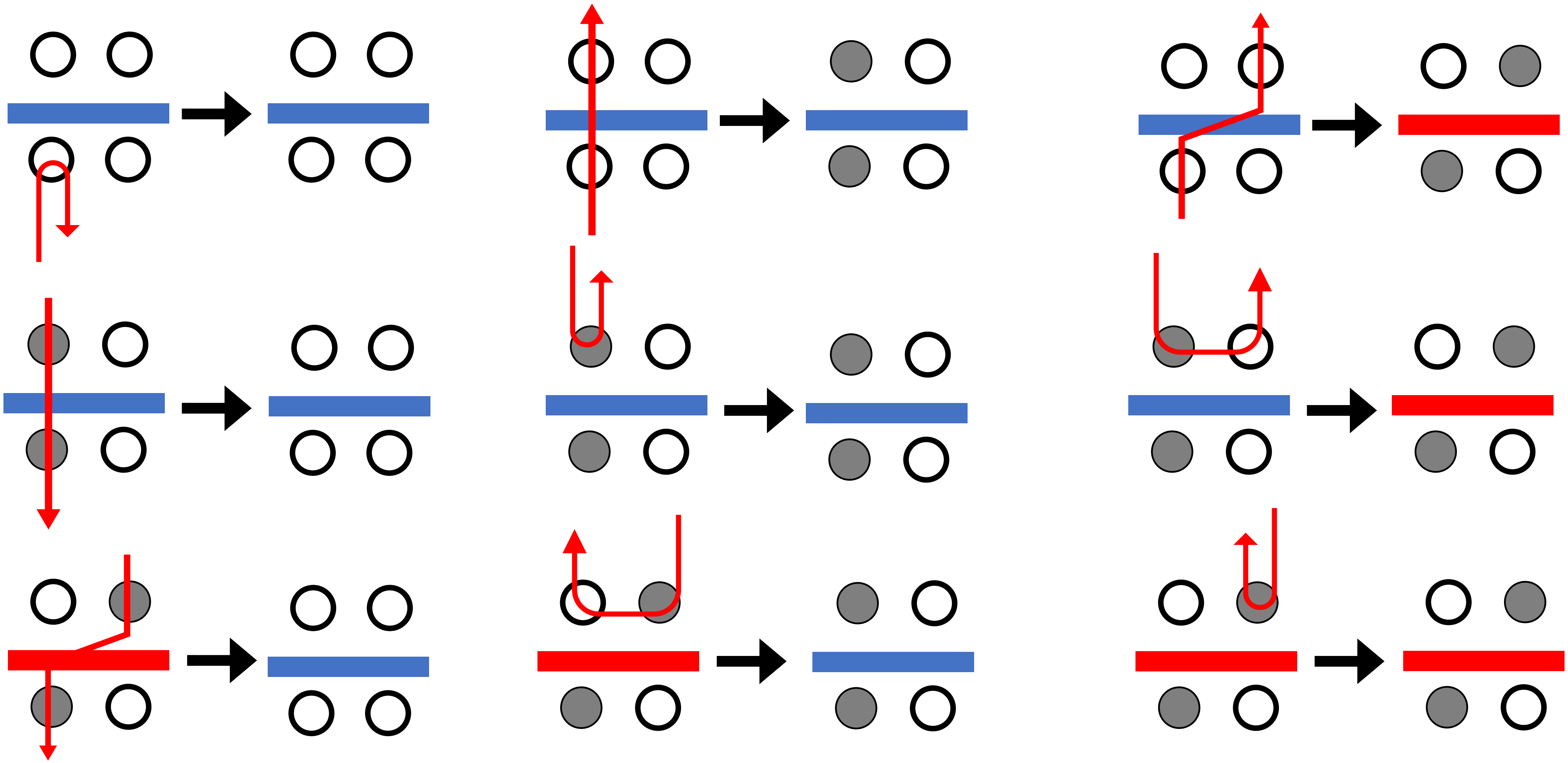
All the weight > 0

Initialization of transfer matrix

```
#--------Begining of part4 Trans.Probility-------------
# Transmatrix
#Storing the type after transformation,
#trans_matrix(1,number of outtp,inleg,tp)=outtp
#trans_matrix(2,number of outtp,inleg,tp)=outleg
trans_matrix=-ones(Int,2,3,4,6);
#The vertexes before and after the transformation
invtx=zeros(Int,4);outvtx=zeros(Int,4);
for tp=1:6
    invtx[:]=vtx[tp,:];
    for inleg=1:4
        np=0; #number of possible outtp
        for outleg=1:4
            if inleg==outleg  #bounce
                np=np+1;
                trans_matrix[1,np,inleg,tp]=tp;
                trans_matrix[2,np,inleg,tp]=outleg;
            else
                outvtx[:]=invtx[:];
                #flip the spin
                outvtx[inleg]=1-outvtx[inleg];
                outvtx[outleg]=1-outvtx[outleg];
                outtp=vtx_rev[outvtx[1]*2+outvtx[2]+1,outvtx[3]*2+outvtx[4]+1];
                if outtp≠0  #possible configuration
                    np=np+1;
                    trans_matrix[1,np,inleg,tp]=outtp;
                    trans_matrix[2,np,inleg,tp]=outleg;
                end
            end
        end
    end
end
```



Initialization of transfer probability



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Initialization of transfer probability

```
#The possibility or acceptibility of transfermation
trans_prob=zeros(3,4,6)
w=zeros(3);is_p=0;   #is_p is the index of tp
for tp=1:6
    for inleg=1:4
        for i=1:3
            outtp=trans_matrix[1,i,inleg,tp];
            if outtp==tp
                global is_p=i;
            end
            w[i]=weight[outtp];
        end
        #The order of the weight w
        wo=sortperm(w,rev=true);
        #The ordered weight
        wl=w[wo];
         #The matrix a used for calculating the possibility
        a=zeros(3,3);
        if wl[1]>(wl[2]+wl[3])
            a[1,1]=wl[1]-(wl[2]+wl[3]);
            a[1,2]=wl[2];a[2,1]=a[1,2];
            a[1,3]=wl[3];a[3,1]=a[1,3];
        else
            a[1,2]=(wl[1]+wl[2]-wl[3])/2;a[2,1]=a[1,2];
            a[1,3]=(wl[1]+wl[3]-wl[2])/2;a[3,1]=a[1,3];
            a[2,3]=(wl[2]+wl[3]-wl[1])/2;a[3,2]=a[2,3];
        end
        worev=invperm(wo)
        for i=1:3
            trans_prob[i,inleg,tp]=a[worev[is_p],worev[i]]/w[is_p];
        end
    end
end
#--------End of part4 Trans.Probility----------------
```

$$P_{ij} = \frac{a_{i,j}}{W_i}$$

山西大学学报(自然科学版)45(3):734—743,2022
Journal of Shanxi University(Nat. Sci. Ed.)

DOI:10.13451/j.sxu.ns.2022025

量子蒙特卡洛模拟——随机级数展开方法

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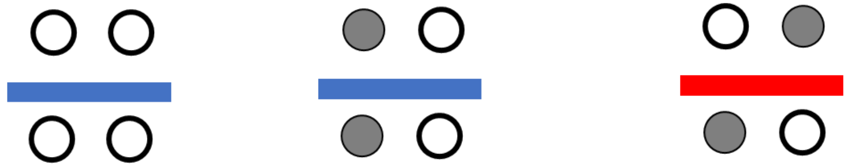
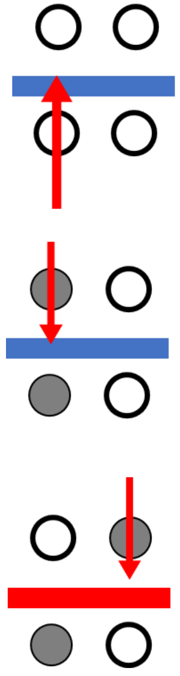


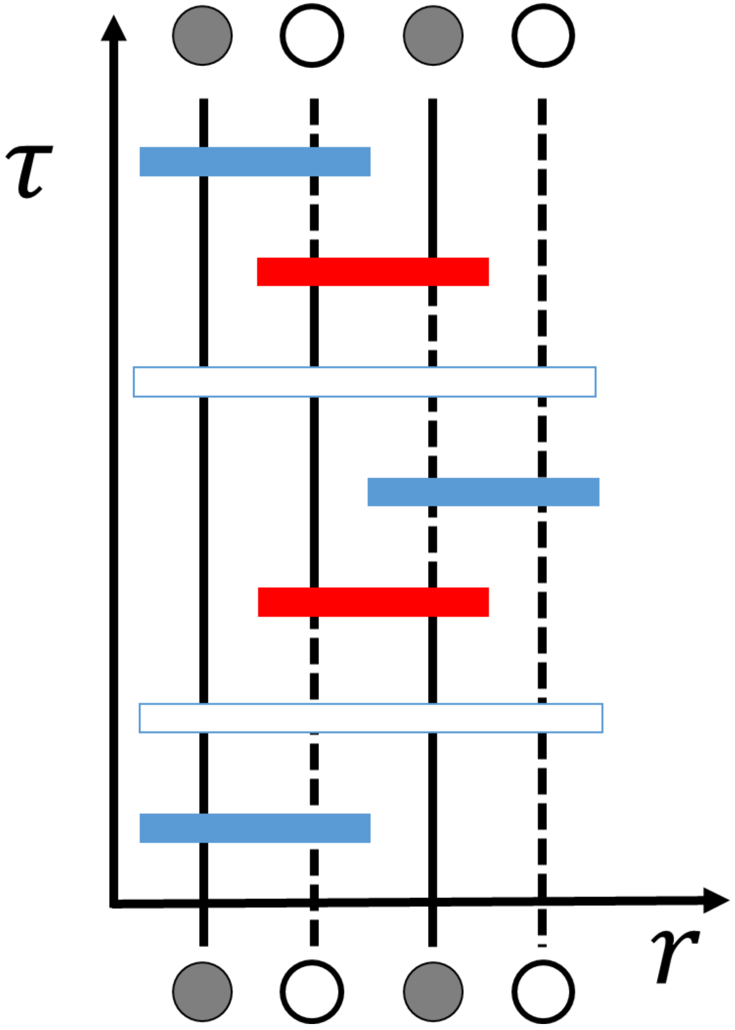


$$a_{1,1} + a_{1,3} + a_{1,6} = W_1$$

$$a_{3,1} + a_{3,3} + a_{3,6} = W_3$$

$$a_{6,1} + a_{6,3} + a_{6,6} = W_6$$

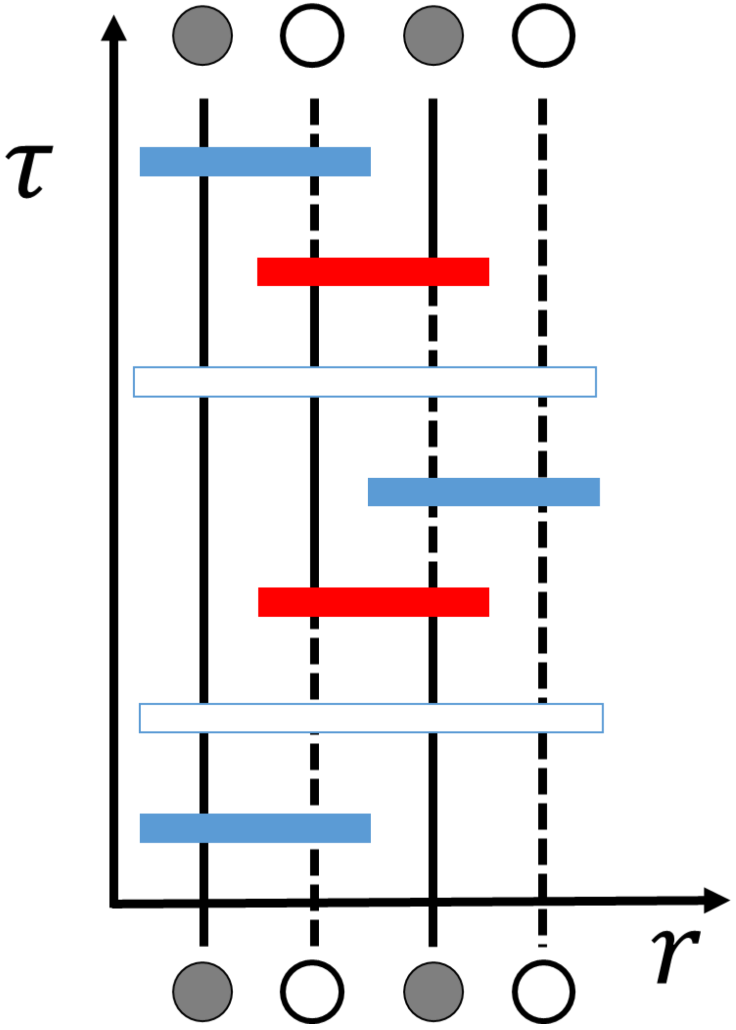
Operator list



Unit Operators (Zero-operator)

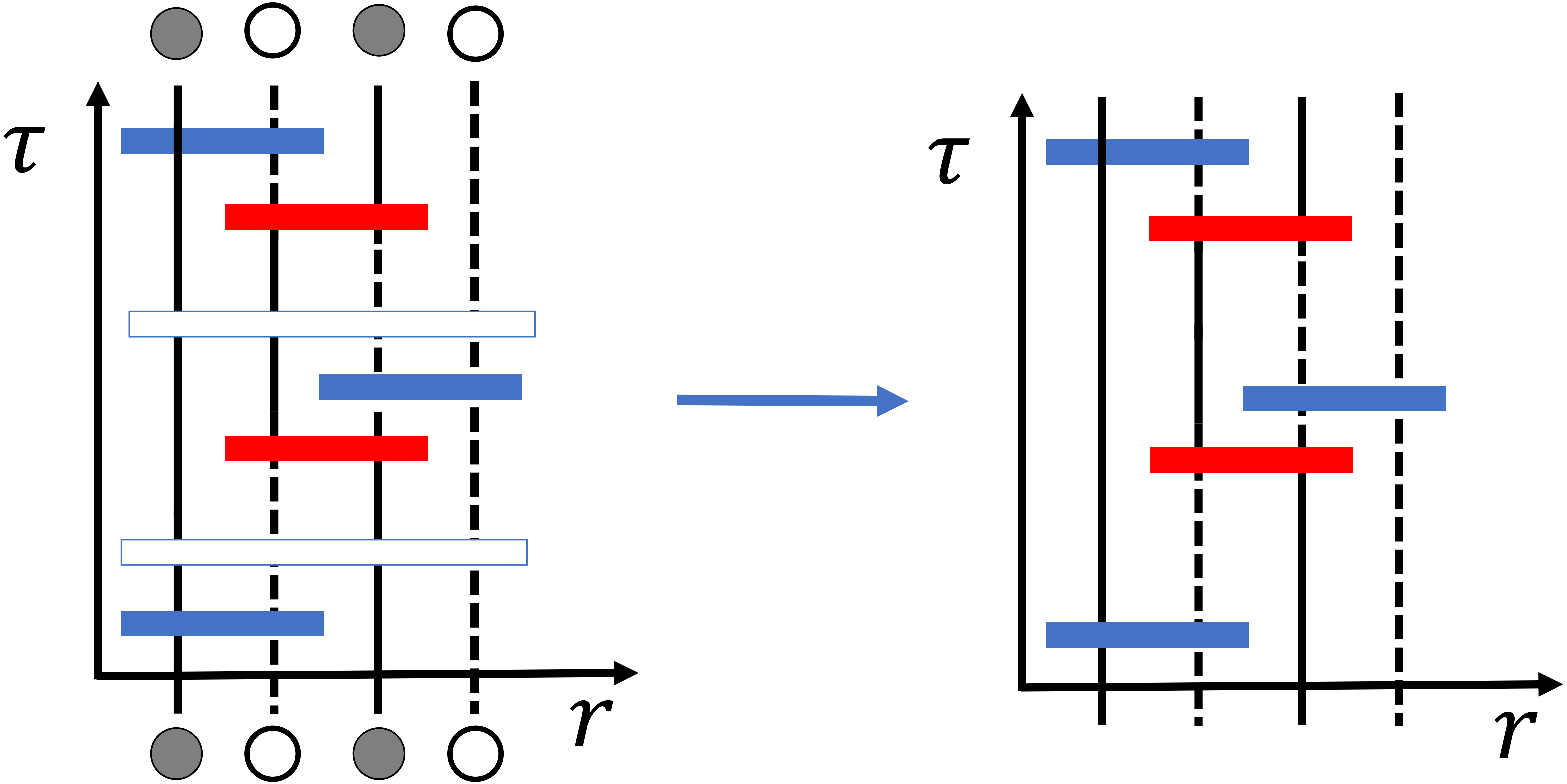
```
#--------Begining of part5 Initial operator list-----
# Initialization of the operator list
#The length for storing the operator list
ll=floor(Int,beta*nb*10);
#The truncation number lm
lm::Int=10;
#The nubmer of non-zero operators,
#there is no non-zero operators at beginning
nh::Int=0;
#The operator list, index 1 store the type of vertex
#index 2 store the position  of operator
#(0 means zero operator)
opl=zeros(Int,2,ll);
#--------End of part5 Trans.Probility---------------
```

Diagonal update

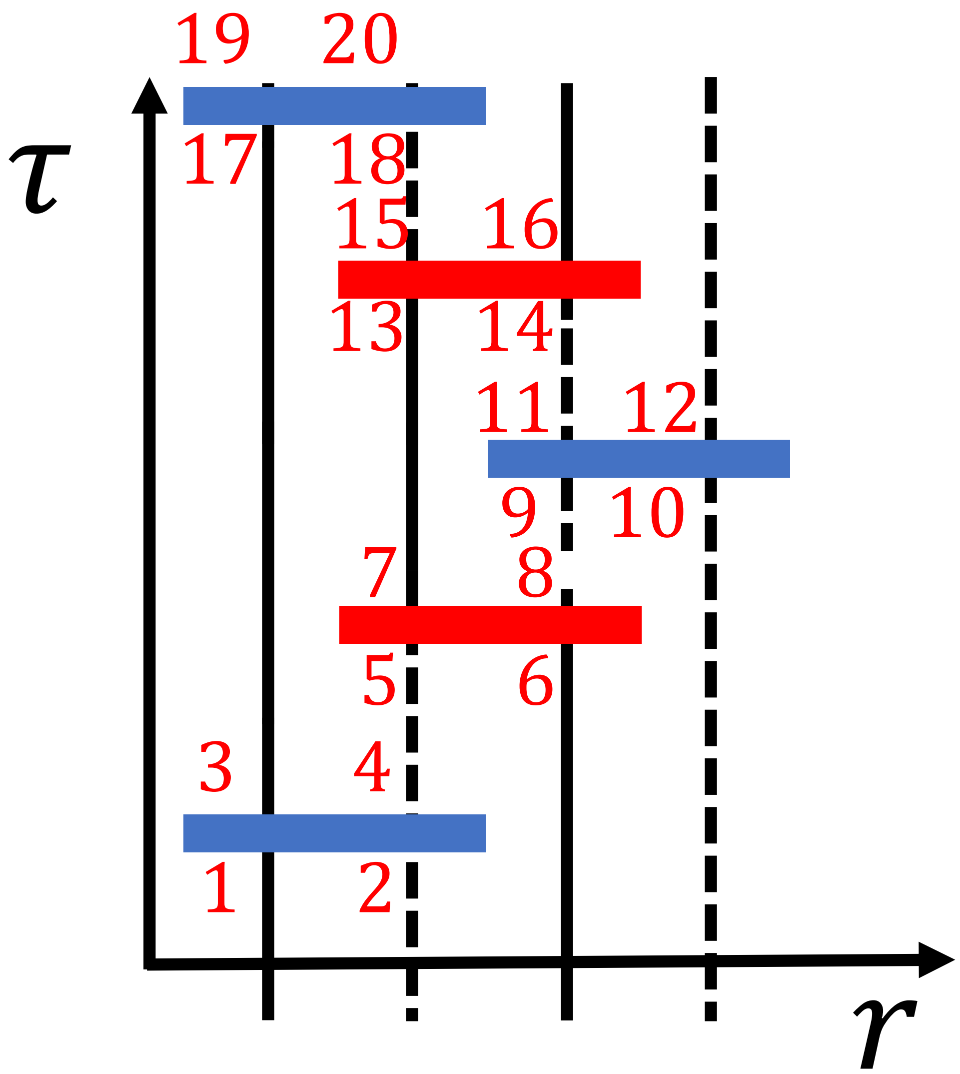



```
function dupdate()
for i=1:lm
    #The type of the vertex
    vtp=opl[1,i];
    if vtp==0                #zero operator
        #select one random position
        r=min(floor(Int64,rndm()*nb),nb-1)+1;;
        #The type of vertex
        tp=conf[bond[1,r]]*2+conf[bond[2,r]]+1;
        ap=(weight[tp]*beta*nb)/(lm-nh); #The probability
        if ap>rndm()    #zero -> non-zero
            #storing the vertex information into the operator list
            opl[1,i]=tp;opl[2,i]=r;
            #non-zero operator plus one
            global nh=nh+1;
        end
    elseif vtp<5            #diagonal operator
        ap=(lm-nh+1)/(weight[vtp]*beta*nb);
        if ap>rndm()    #nonzero -> zero
            #ereasing the vertex information
            opl[1,i]=0;opl[2,i]=0;
            #non-zero operator minus one
            global nh=nh-1;
        end
    else            #off-diagonal operator
        r=opl[2,i];
        conf[bond[1,r]]=vtx[vtp,3];
        conf[bond[2,r]]=vtx[vtp,4];
    end
end
```

Link table

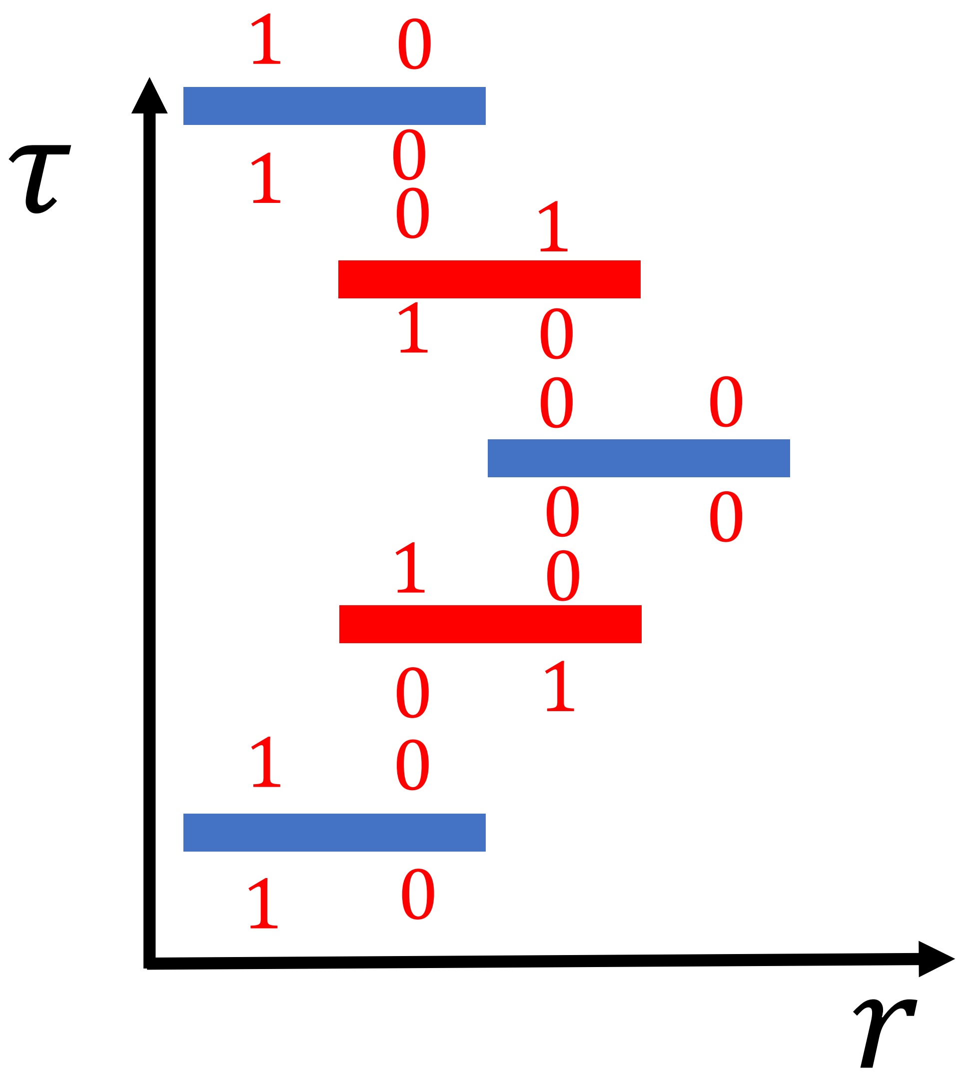


Link table




```
for i=1:lm
    tp=opl[1,i]; #The type of the vertex
    if tp≠0   #Non-zero operator
        is=is+1;opl2[:,is]=opl[:,i];
        r=opl[2,i]; #position of the operator
        for leg=1:2
            bl=bond[leg,r];
            if  ft[bl]==-1; ft[bl]=ln+leg;end
            if  lt[bl]==-1
                lt[bl]=ln+2+leg; #storing the last slide
            else
                 #Link the operator before and after
                link[lt[bl]]=ln+leg;
                link[ln+leg]=lt[bl];
                #move to next slide
                lt[bl]=ln+2+leg;
            end
        end
        ln=ln+4; #Increase the number of legs
    end
end
#After that, link the legs at the boundary
for i=1:ns
    if ft[i]≠-1
        link[ft[i]]=lt[i];
        link[lt[i]]=ft[i];
    end
end
```

Loop update




```
#----------loop starting---------------------------
lplength=0; #loop length
ap=0.;
for i=1:nh*4
    j0=min(floor(Int64,rndm()*nh*4),nh*4-1)+1;  #starting point
    j1=j0;j2=-1;st=0;
    while j2≠j0
        inleg=mod((j1-1),4)+1;
        st=floor(Int,(j1-1)/4)+1;  #position of the vertex
        vtx0=opl2[1,st];
        #choose the outleg
        ap=rndm();w1=trans_prob[1,inleg,vtx0];is=3;
        if ap<w1
            is=1;
        elseif ap<(w1+trans_prob[2,inleg,vtx0])
            is=2;
        end
        vtx2=trans_matrix[1,is,inleg,vtx0];
        outleg=trans_matrix[2,is,inleg,vtx0];
        j2=j1-inleg+outleg;
        opl2[1,st]=vtx2;
        lplength=lplength+1;
        j1=link[j2];
        if j1==j0; break;end
    end
    if lplength>2*nh;break;end
end
```

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Recovering the configuration

```
#recovering the configuration
for i=1:ns
    if ft[i]≠-1
        st=floor(Int,(ft[i]-1)/4)+1;  #position of the operator
        inleg=mod((ft[i]-1),4)+1;
        vtx0=opl2[1,st];
        conf[i]=vtx[vtx0,inleg];
    end
end
    #updating the original operator list
is=0;
    for i=1:lm
        if opl[1,i]≠0
            is=is+1;
            opl[:,i]=opl2[:,is];
        end
    end
end
```

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Main Program

```
#--------Begining of main part -------------
istp=5000;          #The number of thermalization step
mstp=10000;         #The number of Measuring steps
for i=1:istp
    dupdate();
    lupdate();
    lt=floor(Int,1.25*nh);
    if lt>lm
        global lm=lt;
    end
end
    en=zeros(mstp);
    mag=zeros(mstp);
    mag_s=zeros(mstp);
for i=1:mstp
    dupdate();
    lupdate();
    en[i]=nh;
    rho1=sum(conf[1:2:ns]);
    rho2=sum(conf[2:2:ns]);
    mag[i]=rho1+rho2;
    mag_s[i]=(rho1-rho2)^2;
end

display("The Energy is:"*string(sum(en.*1.)/mstp/beta/nb-energy_shift))
display("The magnetization is:"*string(sum(mag.*1.)/mstp/nb))
display("The stagger magnetization is:"*string(sum(mag_s.*1.)/mstp/nb))
```

J. Phys. A: Math. Gen. 25 (1992) 3667–3682. Printed in the UK

A generalization of Handscomb's quantum Monte Carlo scheme—application to the 1D Hubbard model

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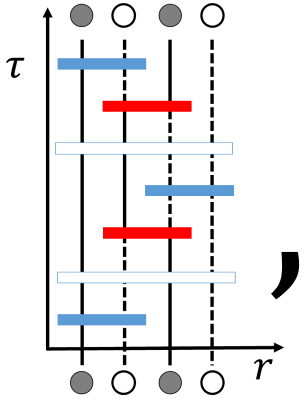
Received 2 January 1992, in final form 30 March 1992

$$E = -\frac{\langle n \rangle_W}{\beta} \qquad M = \left\langle \sum_i S_i^z \right\rangle_W \qquad M_s^2 = \left\langle \left(\sum_{i\in A} S_i^z - \sum_{i\in B} S_i^z \right)^2 \right\rangle_W$$

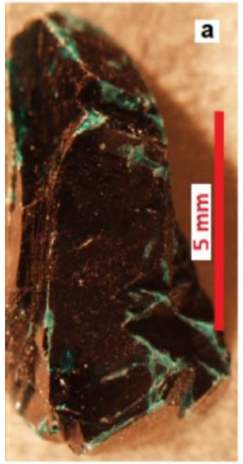
QMC ↔Quantum Material

sampling → $\{$



$, \cdots\ \cdots \}$ Measure → $\{E, M, \rho_S, \chi, S(Q), \ldots\}$

sample → $\{$



$, \cdots\ \cdots \}$ Measure → {ARPES, NMR, STM, … }

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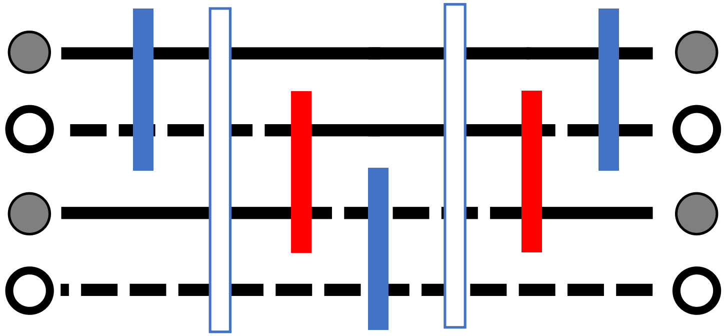
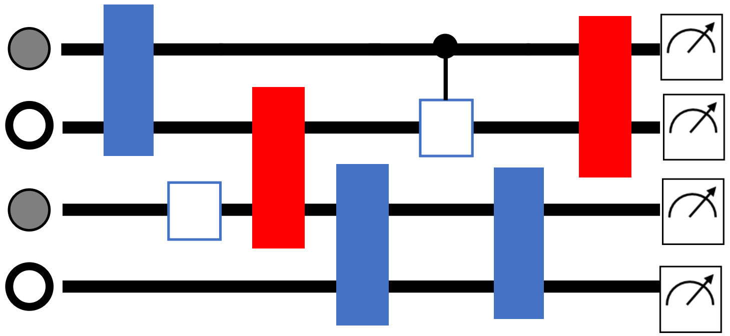
QMC↔Quantum Computing

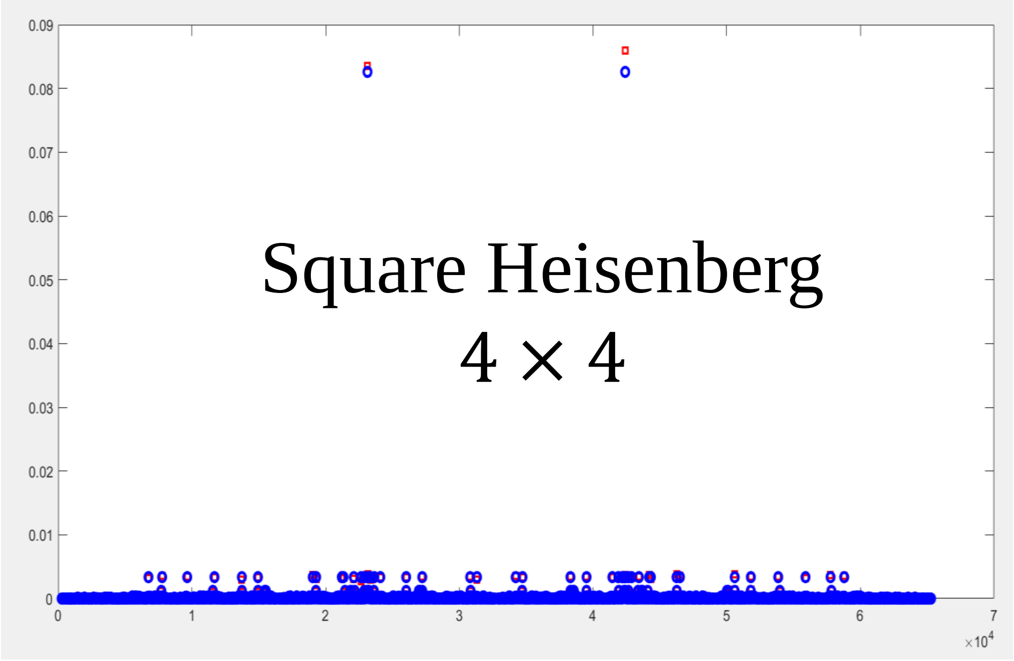
sampling



$\rho_{\alpha,\alpha}|\alpha\rangle\langle\alpha|$ $\langle\alpha|=1010$

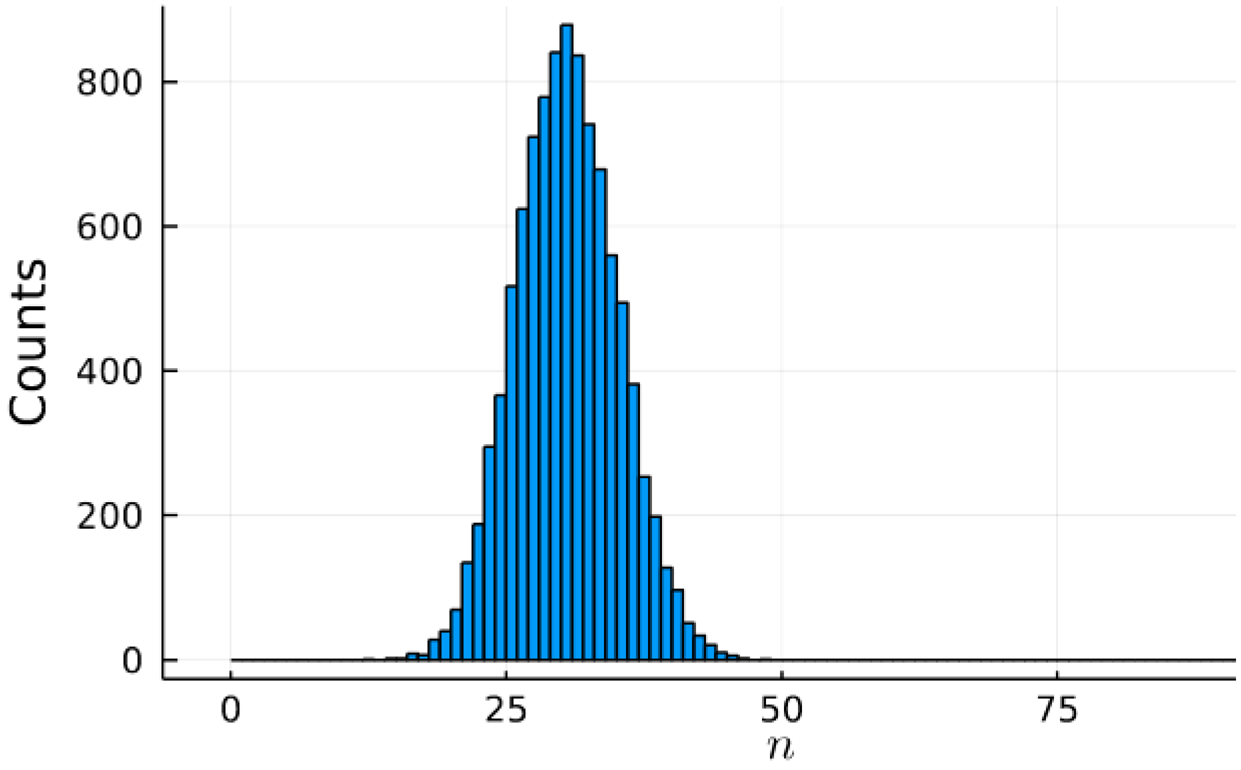
$$\rho_{\alpha,\alpha} = \langle\alpha|\exp(-\beta H)\,|\alpha\rangle \xrightarrow[\lim\ \beta\to+\infty]{} = |\langle\alpha|\phi_0|\alpha\rangle|^2$$



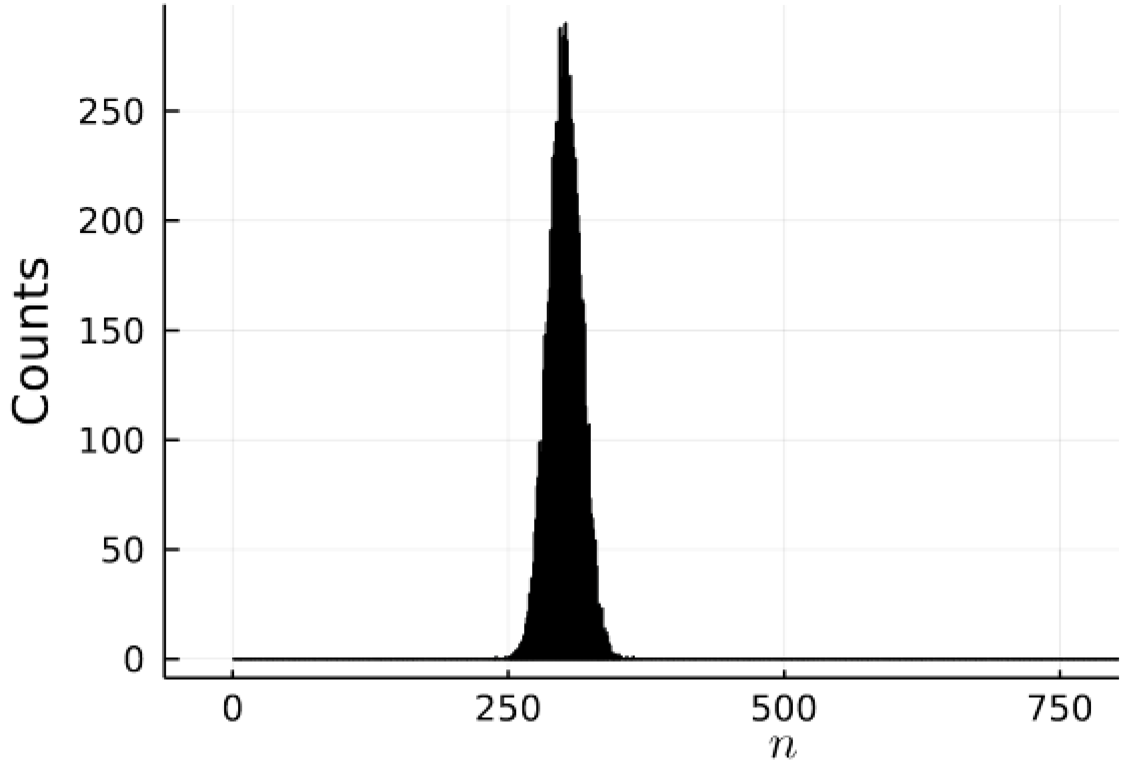


Measure

```
# Launch the sampling
N=100;bin=10000;
histogram(dis(bin,N),bins=0:N,legend=:false,size=(480,270))
xlabel!("\$n\$");ylabel!("Counts")
```

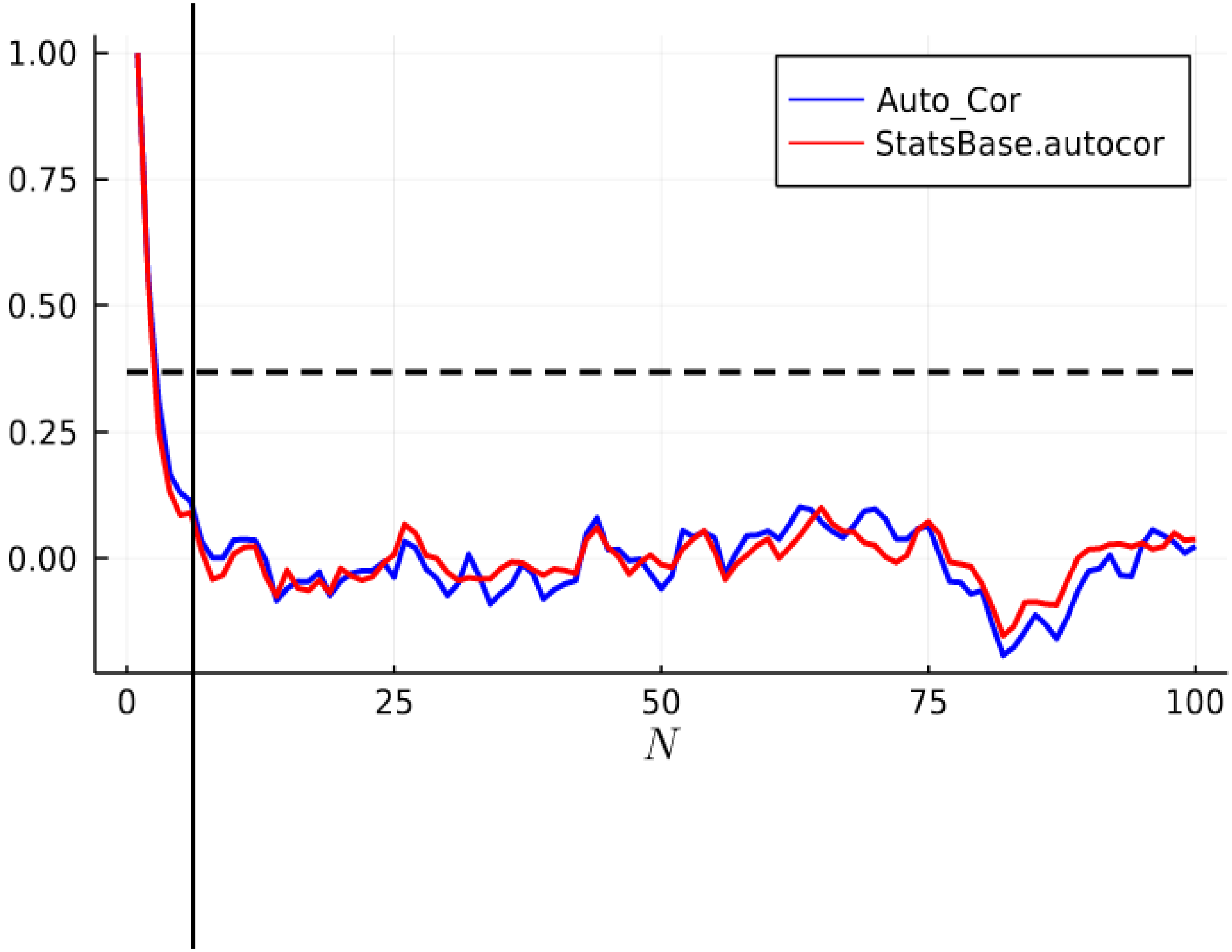



```
# Sampling with more times
N=1000;bin=10000;histogram(dis(bin,N),bins=0:N,legend=:f
xlabel!("\$n\$");ylabel!("Counts")
```



Data Analysis

```
function auto_cor(data,nd)
    ln=floor(Int,nd/2);      #Length of the
    cor=zeros(Float64,ln+1);
    len=1:ln;
    datat=data.-sum(data)/nd;
    xt=datat[len];
    for t=0:ln
        cor[t+1]=dot(xt,datat[t.+len]);
    end
    cor=cor./ln;
    return cor
end;
```



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Data Analysis

ADVANCES IN PHYSICS, 2003, VOL. 52, NO. 1, 1–66

Taylor & Francis
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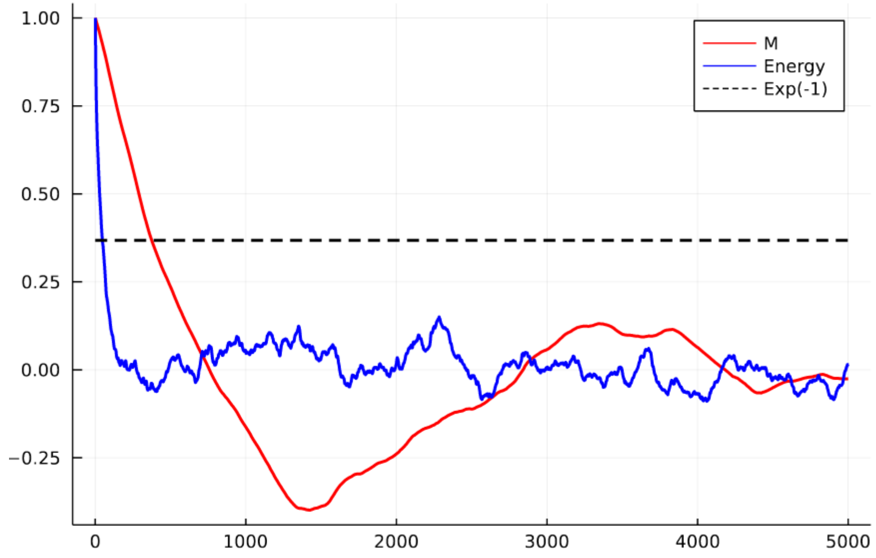
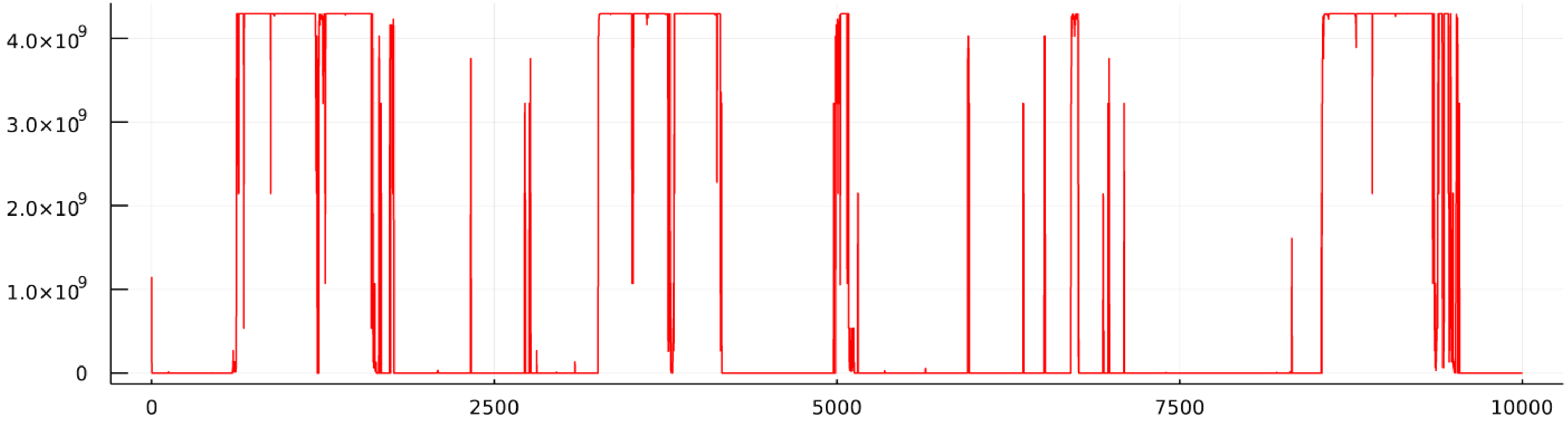
The loop algorithm

H. G. EVERTZ

Institut für Theoretische Physik, Technische Universität Graz, 8010 Graz, Austria;





Data Analysis

```
# Binning method to get the expectation value and error
function finderro(data,bin)
    # Set the value of the bin, group the data;
    ln=length(data);
    k=Int(ln/bin);
    data_new=reshape(data,bin,k);
    datab=vec(sum(data_new,dims=1)./bin);
    ex=sum(datab)/k;          #Expectation value
    datab=datab.-ex;
    var=sum(datab.*datab)/k;      #Variance    \sigma^2
    d_err=sqrt(var/k);
    return ex,d_err
end;
```

Jackknife

Split the measured values $O(i)$ into k groups of length $l = n/k$. To obtain the asymptotic error, l must be significantly larger than the relevant autocorrelation time. Now perform the complete, possibly highly nonlinear, analysis of the MC data $k+1$ times:first with all $l \times k$ data, leading to a result $R^{(0)}$, then, for $j = 1, \ldots, k$, with all data except those in bin j (i.e. pretend that bin j was never measured), leading to values $R^{(j)}$. Then the overall result R is $R = R^{(0)} - Bias$, where $Bias = (k-1)(R^{av} - R^{(0)})$, and $R^{av} = \sum_{j=1}^{k} R^{(j)}/k$. The statistical error is

$$\delta(R) = \sqrt{(k-1)(\frac{1}{k}\sum_{j=1}^{k}(R^{(j)})^2 - (R^{av})^2)}$$

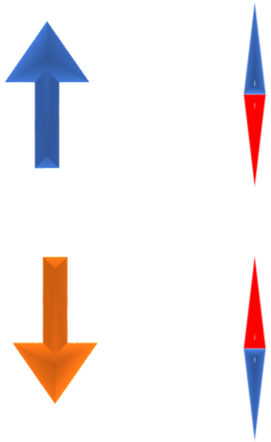
Quantum Magnetism

Ising Model

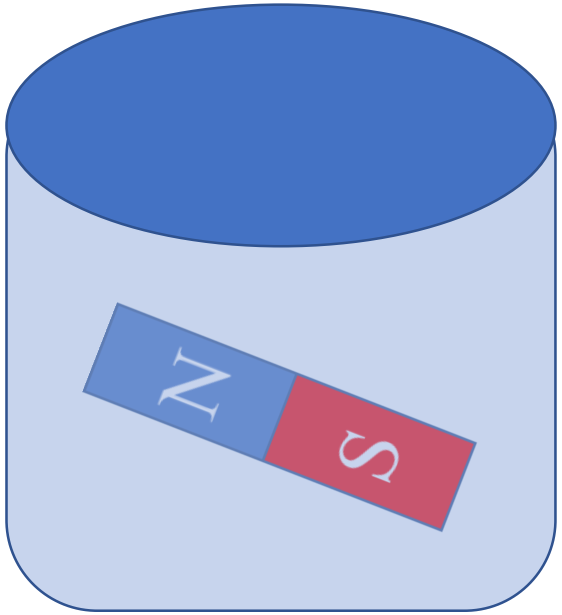
Ising Model:

$$H = J\sum_{\langle i,j\rangle}\sigma_i^Z\sigma_j^Z - B\sum_i \sigma_i^Z$$

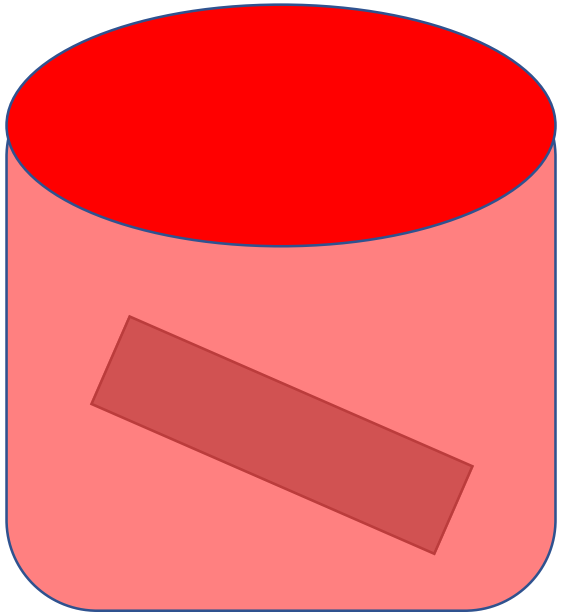
$$\sigma_i^Z = \begin{cases} 1 \\ -1 \end{cases}$$



Ferromagnet



Paramagnet



Heisenberg Model

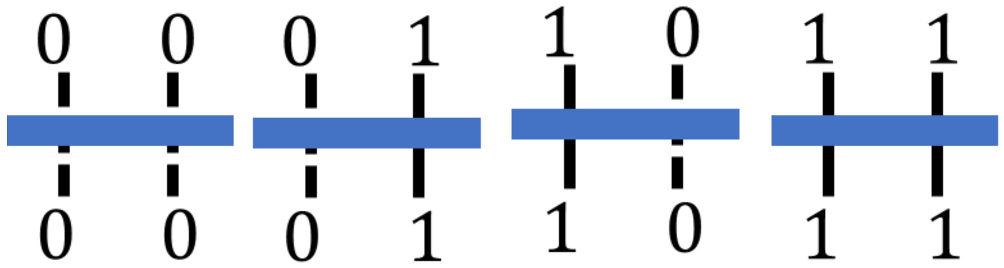
$$H = J\sum_{\langle i,j\rangle} \boldsymbol{S}_i\boldsymbol{S}_j - B\sum_i S_i^Z$$

For spin-1/2: $\boldsymbol{S}_i = \frac{1}{2}\boldsymbol{\sigma}_i$

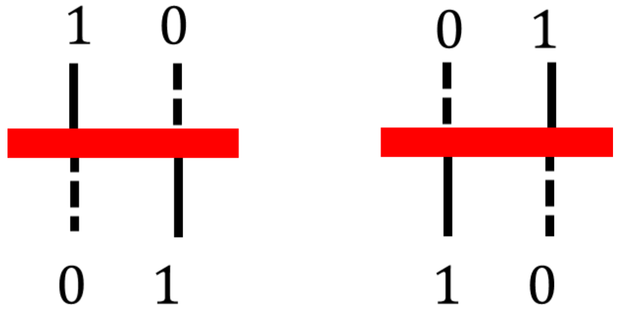
$$H = J\sum_{\langle i,j\rangle}\left(S_i^xS_j^x + S_i^yS_j^y + S_i^zS_j^z\right) - B\sum_i S_i^Z$$

$$= \frac{J}{2}\sum_{\langle i,j\rangle}\left(S_i^+S_j^- + h.c.\right) + J\sum_{\langle i,j\rangle} S_i^zS_j^z - B\sum_i S_i^Z$$

$$J\sum_{\langle i,j\rangle} S_i^zS_j^z - B\sum_i S_i^Z - \delta < 0$$



$$\frac{J}{2}\sum_{\langle i,j\rangle}\left(S_i^+S_j^- + h.c.\right) > 0$$ Sign Problem?



$$S_i^x \xrightarrow{i\in A} -S_i^x$$

$$S_i^y \xrightarrow{i\in A} -S_i^y$$

$$S_i^z \xrightarrow{i\in A} S_i^z$$

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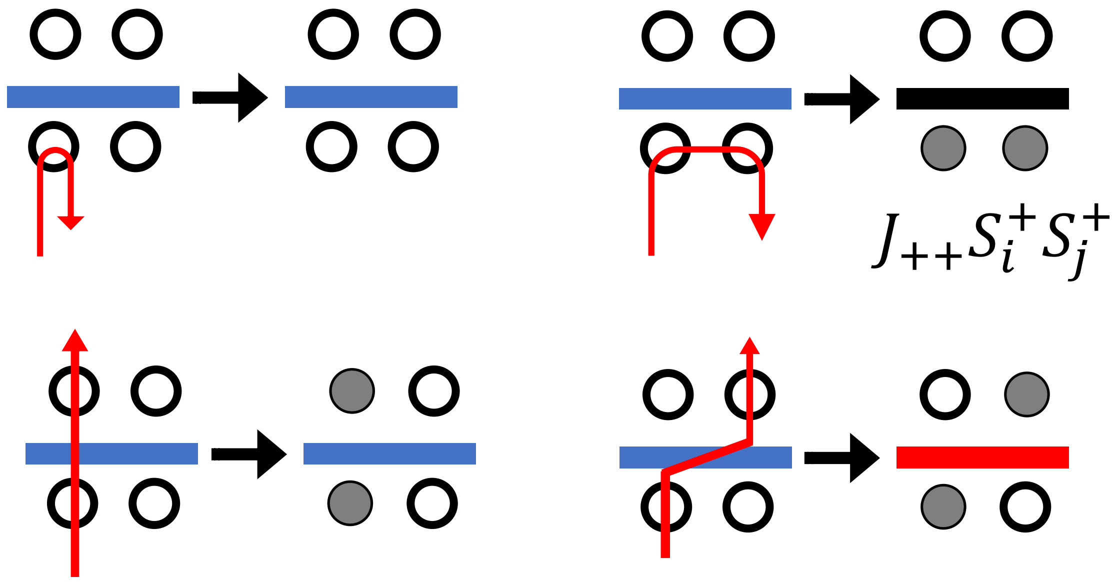
XYZ Model

$$H = J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \boldsymbol{S}_j - B \sum_i S_i^Z$$

For spin-1/2: $\boldsymbol{s}_i = \frac{1}{2} \boldsymbol{\sigma}_i$

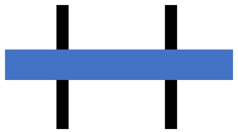
$$H = -\sum_{\langle i,j \rangle} \left(J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_z S_i^z S_j^z \right) - \sum_i S_i^Z$$

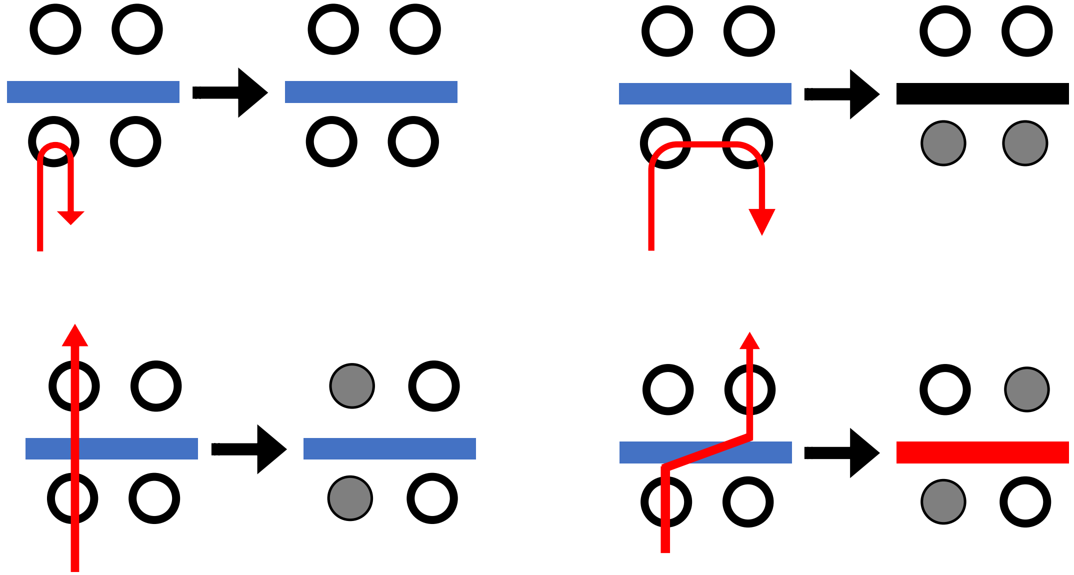
$$= -\sum_{\langle i,j \rangle} \left(J_{\pm} S_i^+ S_j^- + J_{++} S_i^+ S_j^+ + h.c. \right) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z - B \sum_i S_i^Z$$



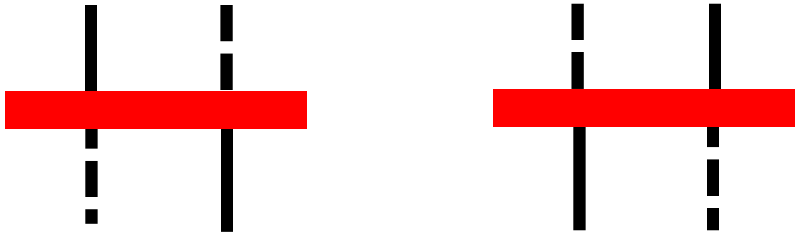
Spin-S Model

Diagonal Operators





Off-Diagonal Operators



$$m = -S, -S+1, \dots, S-1, S$$

$$n = 0, 1, \dots, 2S-1, 2S$$

$$\langle m+1 | S_i^+ | m \rangle = \sqrt{S(S+1) - m(m+1)} = \sqrt{(n+1)(2S-n)}$$

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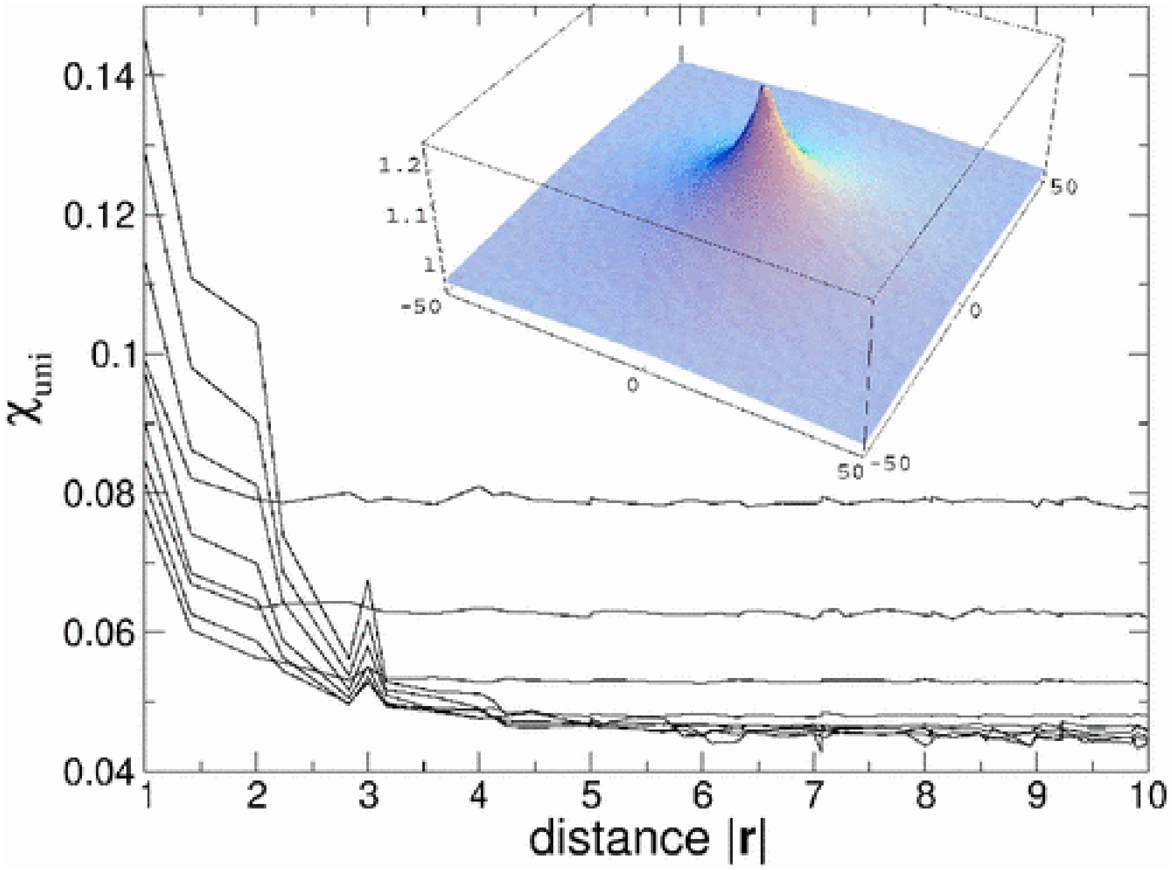
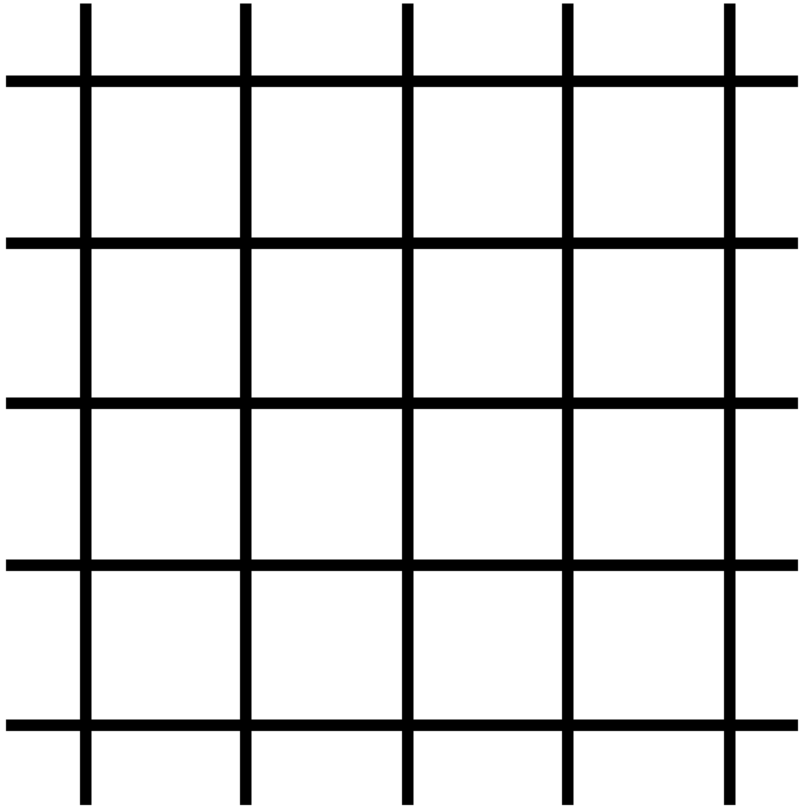
Inhomogeneous Problem

Impurity:



Open boundary:



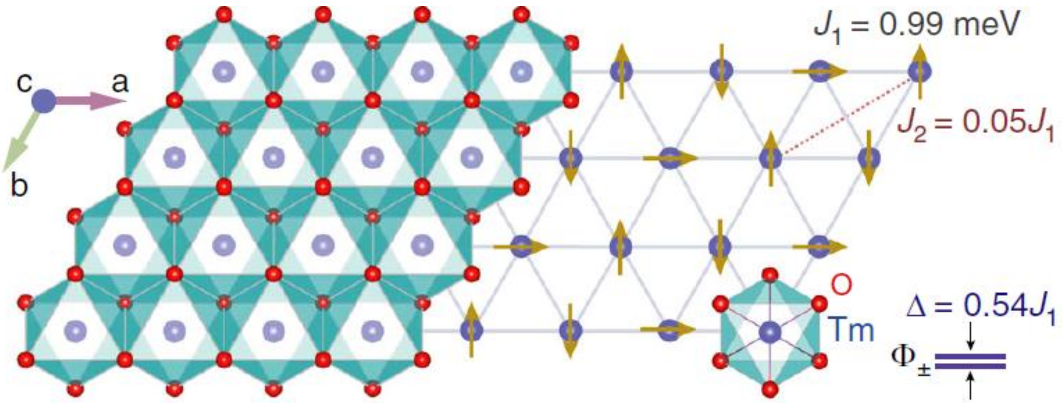
Site dependent vertex and transfer variables: e.g.:   weight[type,nb]

Transverse Ising Model

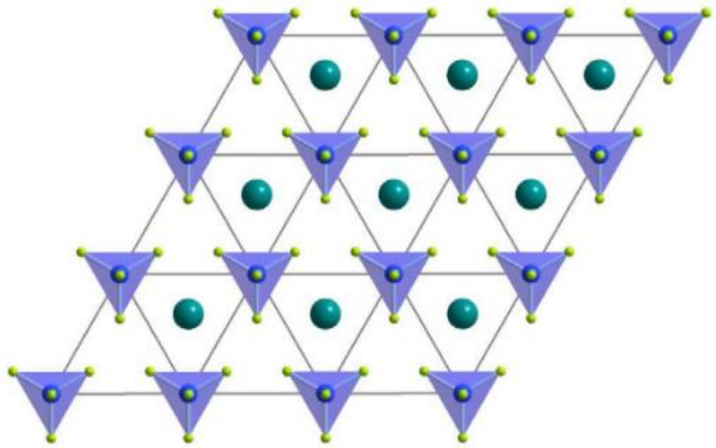
Extended TFIM:

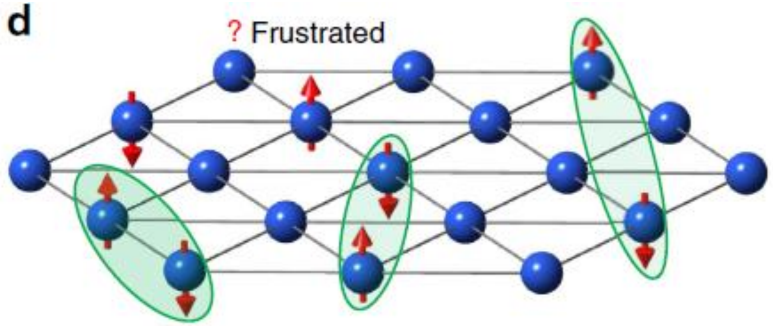
$$H = J_1 \sum_{\langle i,j \rangle} S_i^Z S_j^Z + J_2 \sum_{\langle i,j \rangle} S_i^Z S_j^Z - \Delta \sum_i S_i^x$$

$TmMgGaO_4$ (TMGO)



Paraelectric hexaferrite





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Transverse Ising Model

$$H = J\sum_{\langle i,j\rangle} S_i^Z S_j^Z - \Delta \sum_i (S_i^x + I_i)$$

PHYSICAL REVIEW E **68**, 056701 (2003)

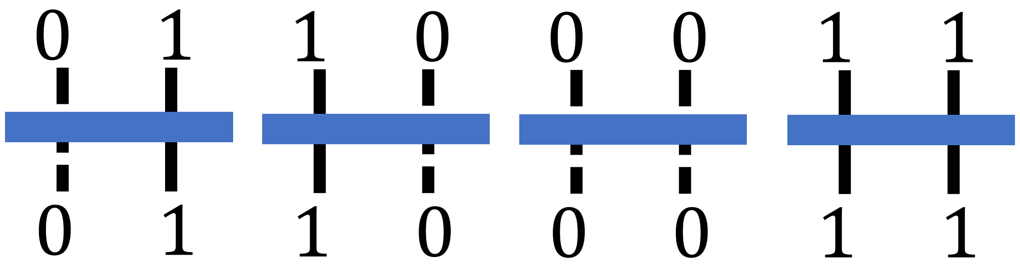
Stochastic series expansion method for quantum Ising models with arbitrary interactions

Anders W. Sandvik
Department of Physics, Åbo Akademi University, Porthansgatan 3, FIN-20500 Turku, Finland

(Received 27 March 2003; published 11 November 2003)

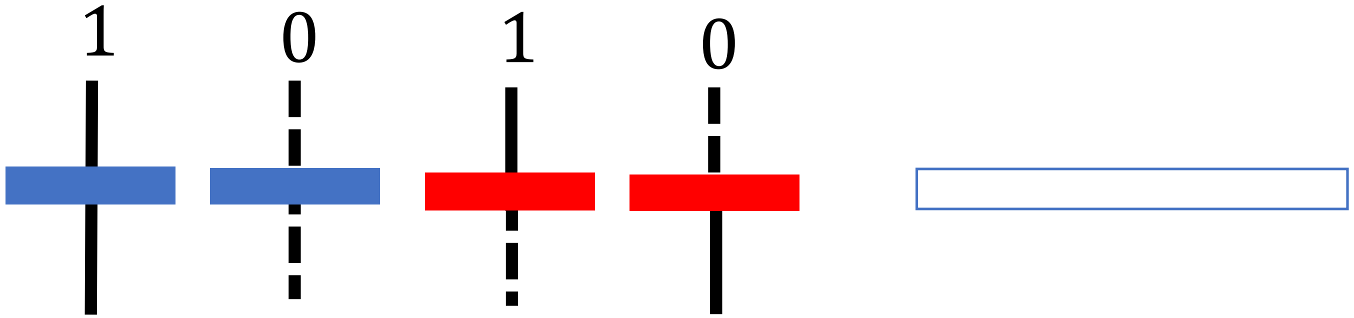
A quantum Monte Carlo algorithm for the transverse Ising model with arbitrary short- or long-range interactions is presented. The algorithm is based on sampling the diagonal matrix elements of the power-series expansion of the density matrix (stochastic series expansion), and avoids the interaction summations necessary in conventional methods. In the case of long-range interactions, the scaling of the computation time with the system size N is therefore reduced from N^2 to $N\ln(N)$. The method is tested on a one-dimensional ferromagnet in a transverse field, with interactions decaying as $1/r^2$.

Diagonal Operators



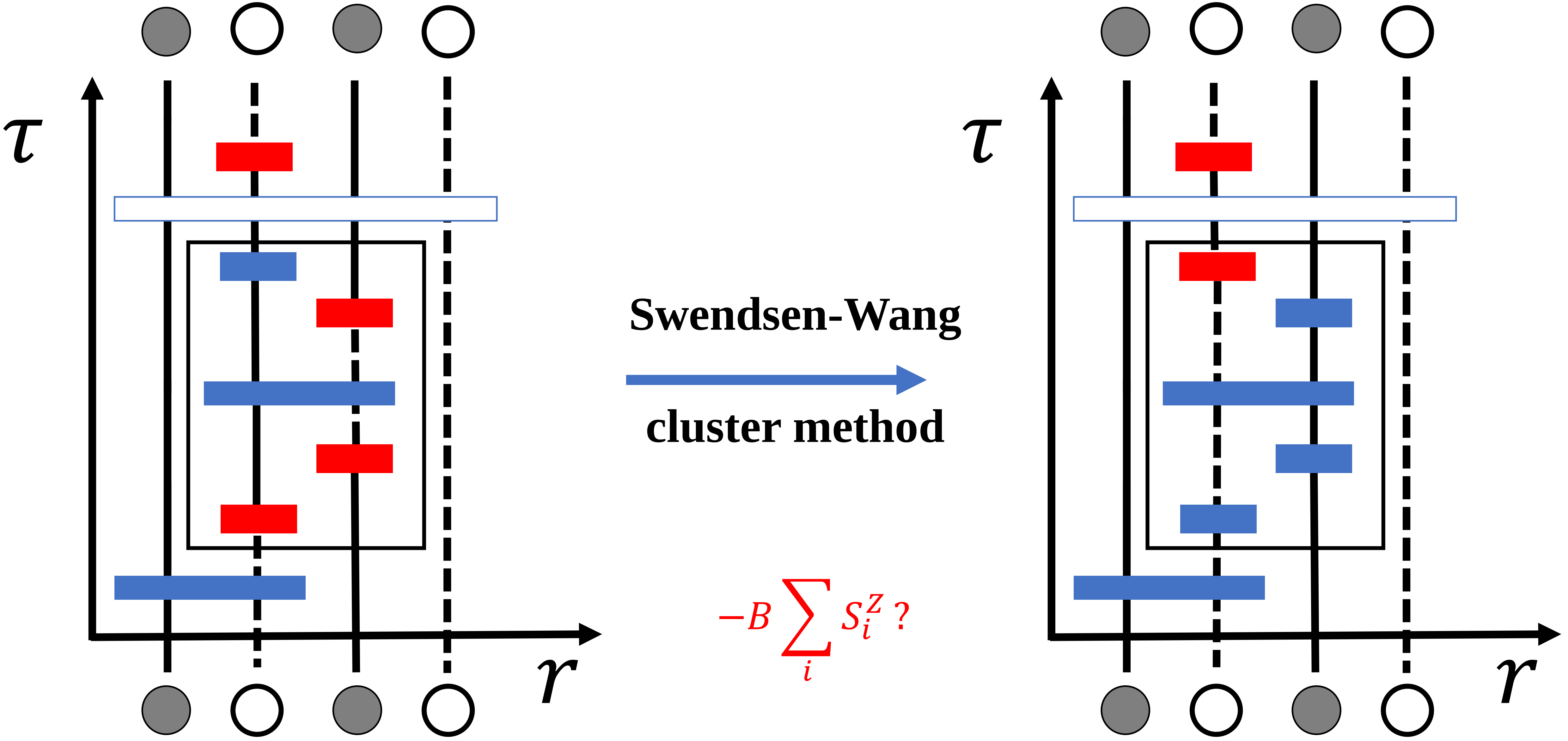
$-\frac{J}{4} \leftrightarrow -\frac{J}{4}$ $\frac{J}{4} \leftrightarrow \frac{J}{4}$

Constants Operators | Off-Diagonal Operators | Unit Operators (Zero-operator)



$\Delta \leftrightarrow \Delta \leftrightarrow \Delta \leftrightarrow \Delta$

Transverse Ising Model



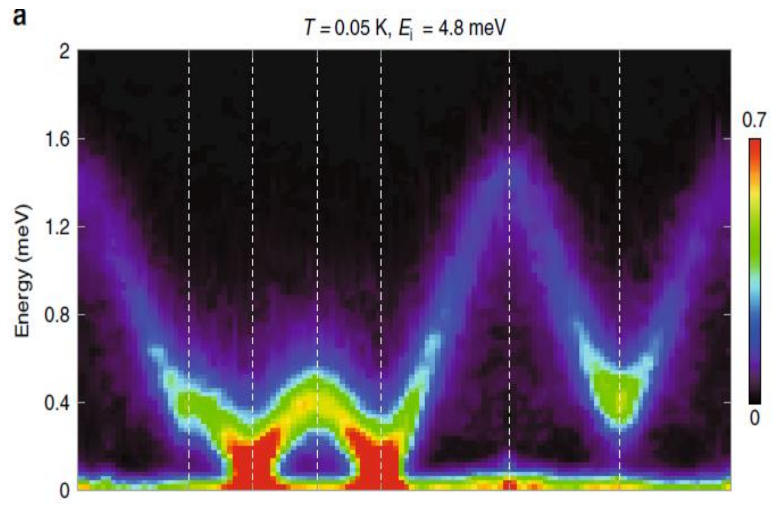
Transverse Ising Model

Dynamical Structure Factor

$$S^{zz}(\boldsymbol{k},\omega) = \frac{1}{2\pi L^2}\sum_{i,j}\int_{-\infty}^{+\infty} dt\, e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)-i\omega t}\langle S_i^z(0)S_j^z(t)\rangle$$

$$S^{+-}(\boldsymbol{k},\omega) = \frac{1}{2\pi L^2}\sum_{i,j}\int_{-\infty}^{+\infty} dt\, e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)-i\omega t}\langle S_i^+(0)S_j^-(t)\rangle$$

$$\left.\begin{array}{l}\langle S_i^z(0)S_j^z(\tau)\rangle \\ \langle S_i^+(0)S_j^-(\tau)\rangle\end{array}\right\} + \mathrm{SAC}$$



2021-10 57(5) 北京师范大学学报(自然科学版) Journal of Beijing Normal University(Natural Science) 593

随机序列展开量子蒙特卡洛模拟中非对角关联函数的测量*

朱文静[1] 郭文安[1]†

(1)北京师范大学物理学系，100875，北京)

+

Physics Reports 1003 (2023) 1–88

Contents lists available at ScienceDire

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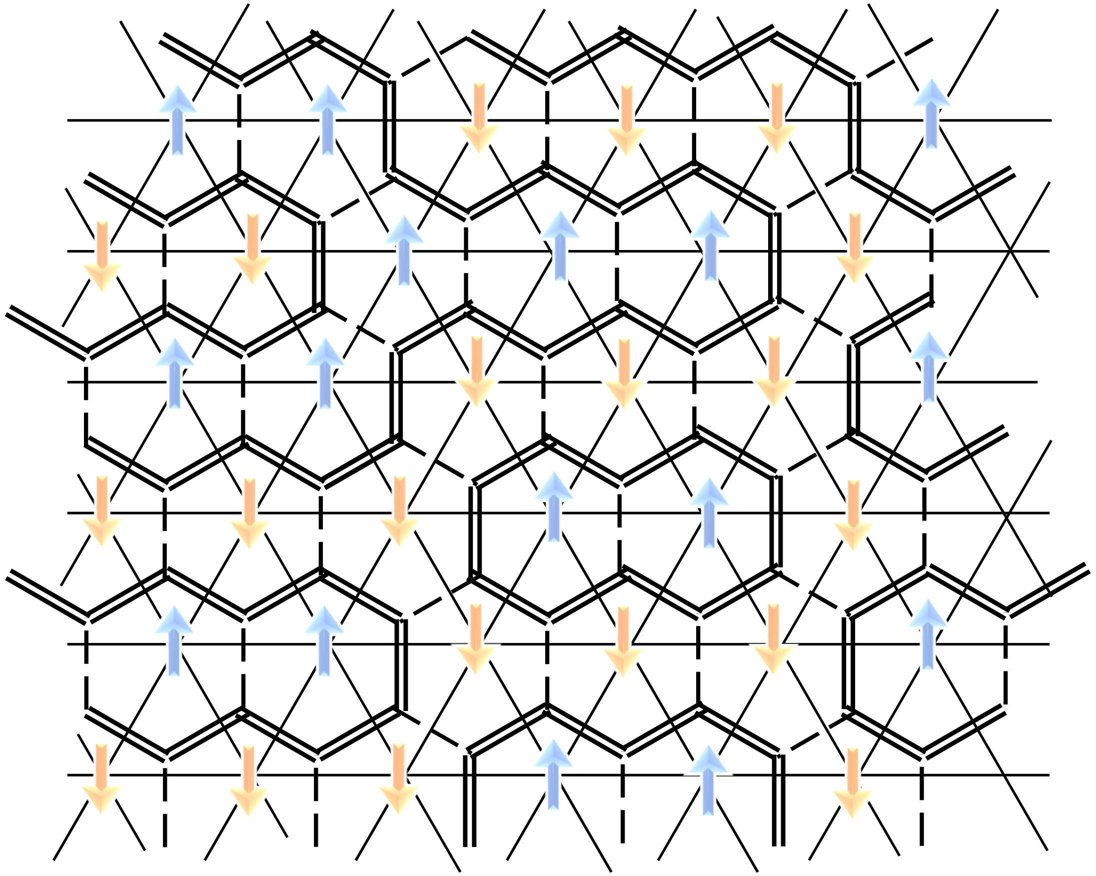
journal homepage: www.elsevier.com/locate

Progress on stochastic analytic continuation of quantum Monte Carlo data

Hui Shao[a], Anders W. Sandvik[b,c,*]

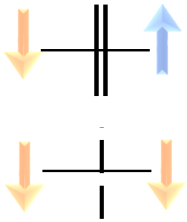
重庆大学
CHONGQING UNIVERSITY

Quantum Dimer model



PBC

Dimer mapping



T. Schlittler, T. Barthel, G. Misguich, J. Vidal, and R. Mosseri,
PRL **115**, 217202 (2015)

Global scheme of sweeping cluster algorithm to sample among topological sectors

Zheng Yan
Phys. Rev. B **105**, 184432 – Published 31 May 2022

$$H_{QDM} = -t\hat{T} + v\hat{V}$$

$$= -t\left(|\nabla\rangle\langle\Delta| + \text{H.c.}\right) + v\left(|\nabla\rangle\langle\nabla| + |\Delta\rangle\langle\Delta|\right)$$

Optical Lattice

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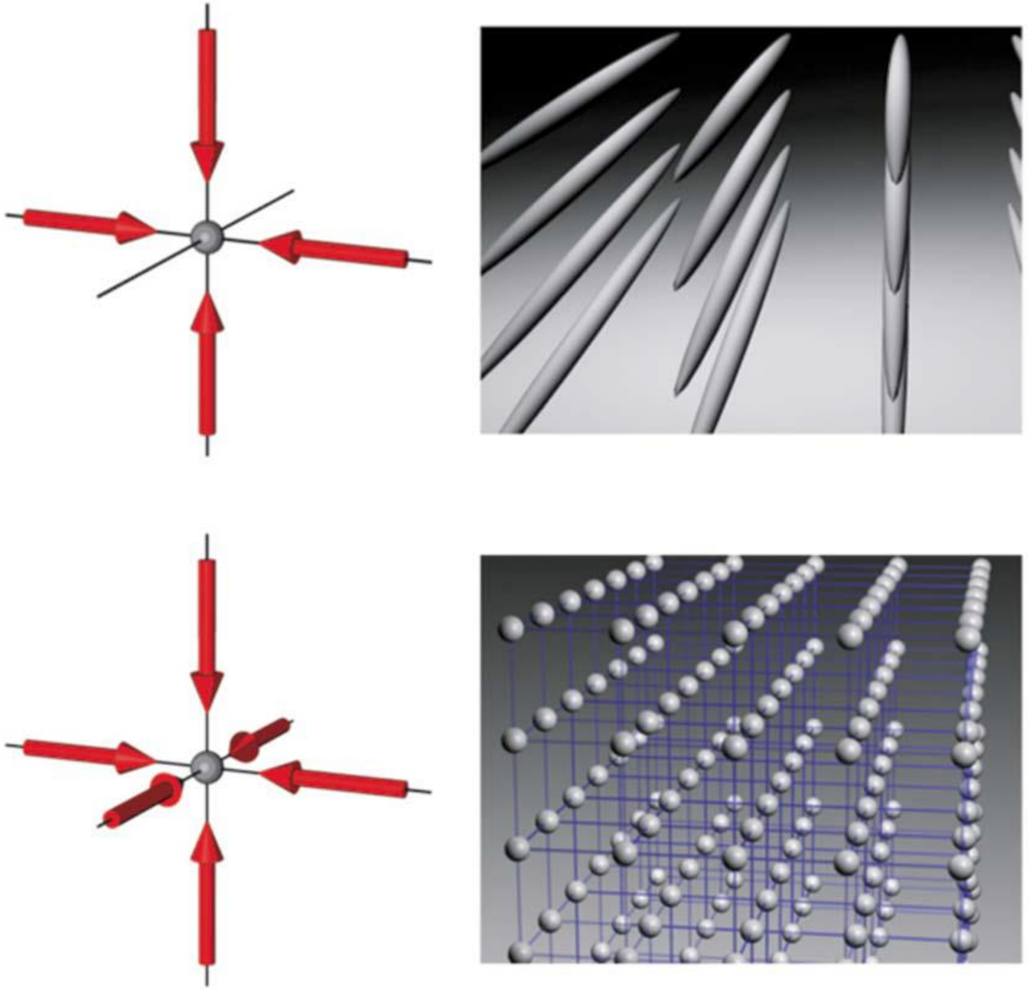
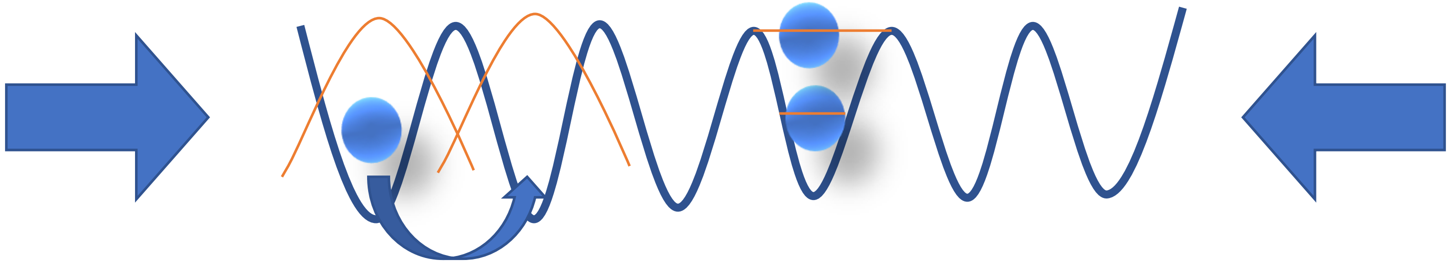
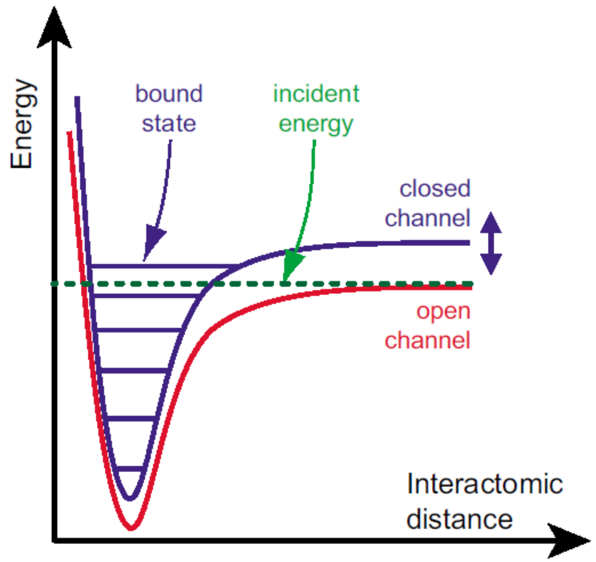
Optical lattice



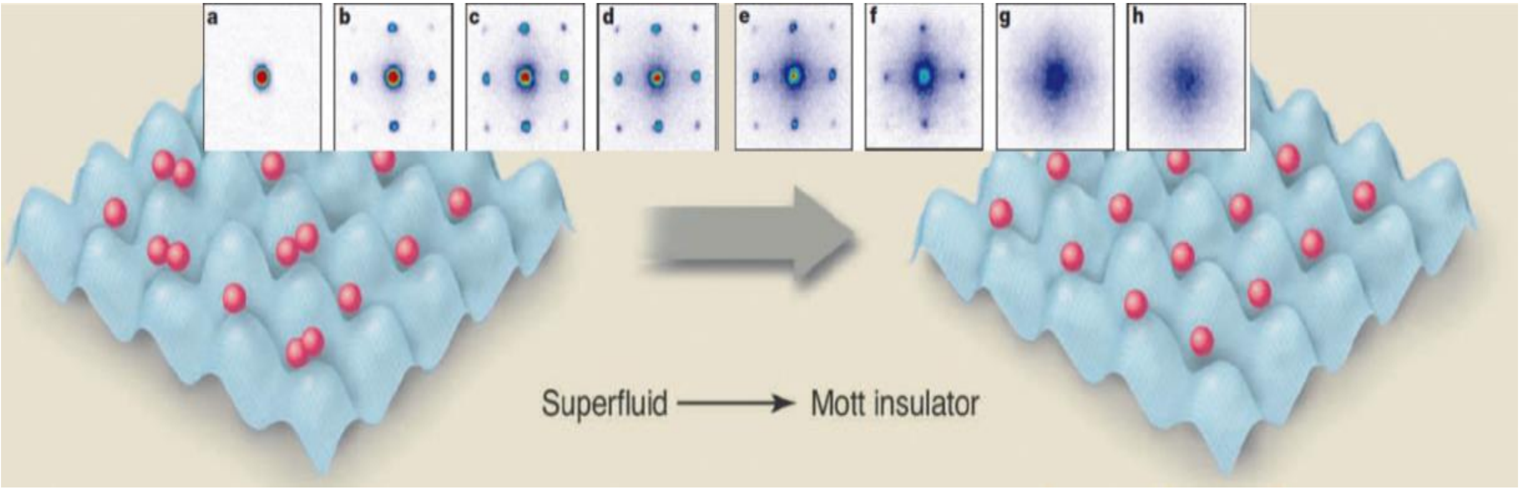
Optical lattice





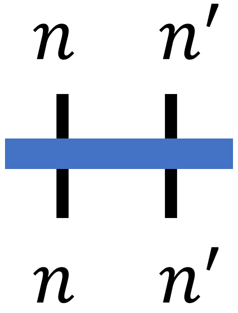
Bose-Hubbard Model

$$H = -t\sum_{i,j}(b_i^{\dagger}b_j + h.c.) + \frac{U}{2}\sum_i n_i(n_i - 1) - \mu\sum_i n_i$$

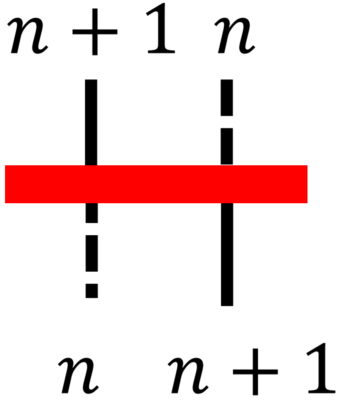


SSE

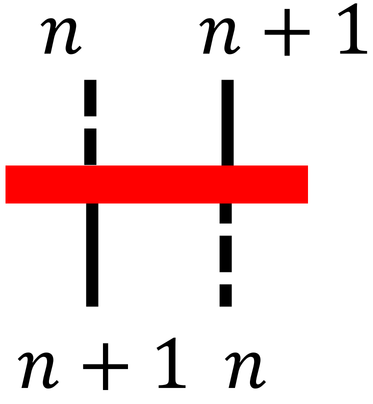
Diagonal Operators



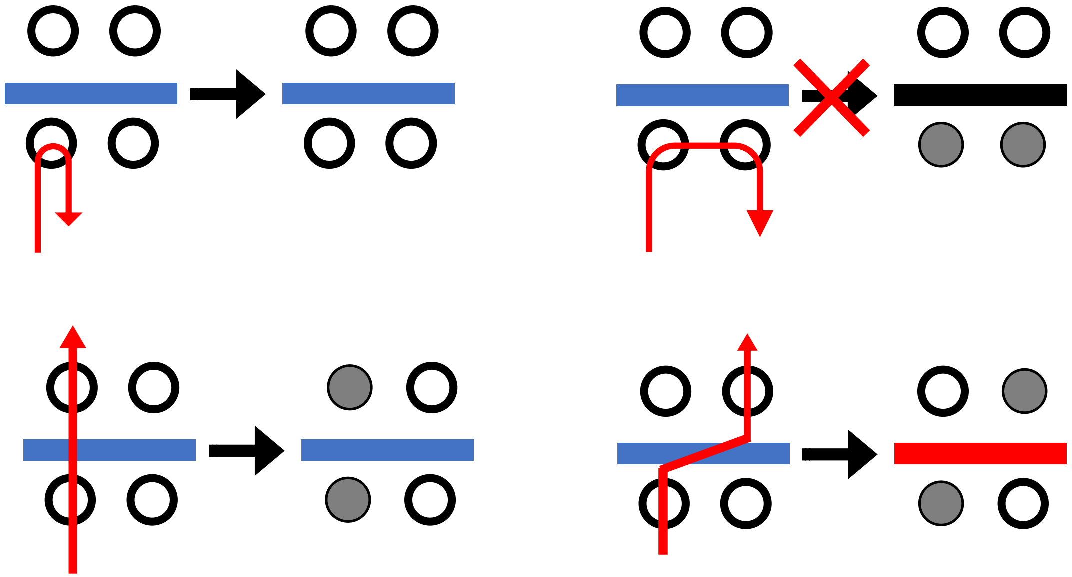
Off-Diagonal Operators



$-t\ b_i^{\dagger} b_j$



$-t\ b_i b_j^{\dagger}$

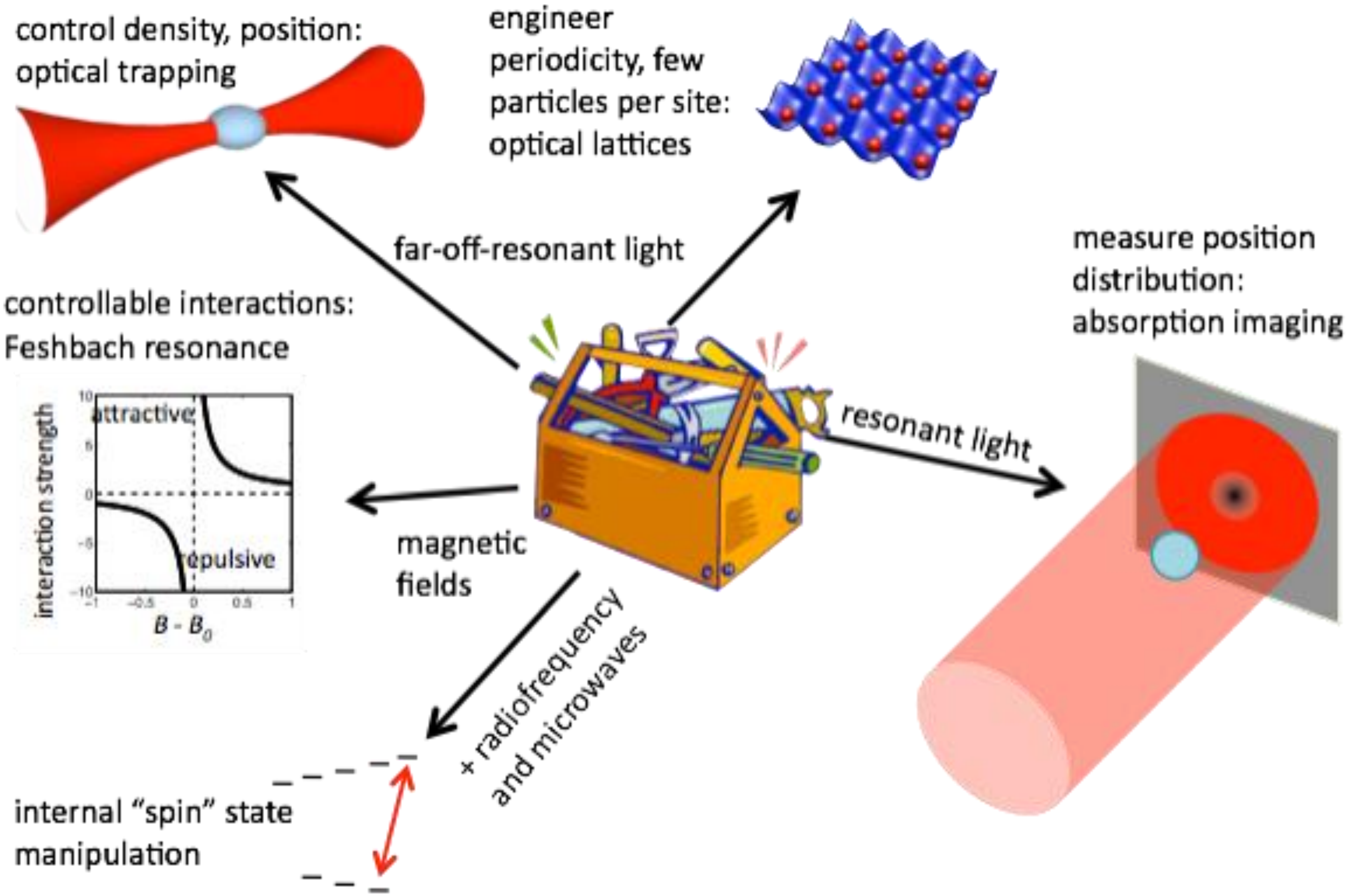


$$n = 0, 1, \ldots, n_{Max}$$

$$\langle n+1 | b_i^{+} | n \rangle = \sqrt{(n+1)}$$

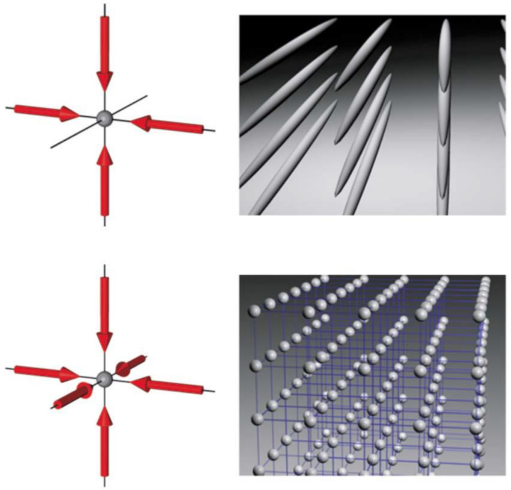
$$\langle n-1 | b_i | n \rangle = \sqrt{n}$$

Tool Box

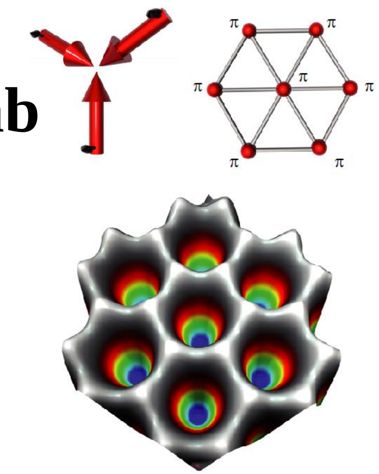

control density, position:
optical trapping
engineer
periodicity, few
particles per site:
optical lattices
far-off-resonant light
measure position
distribution:
absorption imaging
controllable interactions:
Feshbach resonance
attractive
repulsive
interaction strength
B - B0
resonant light
magnetic
fields
+ radiofrequency
and microwaves
internal "spin" state
manipulation

Geometry

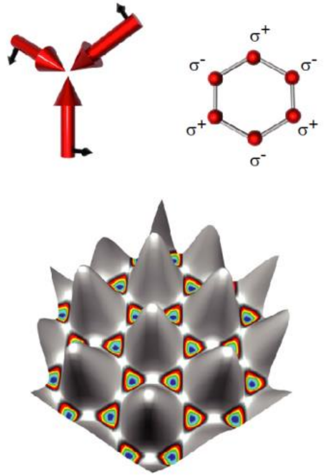
Dimension Crossover:



Honeycomb Lattice:

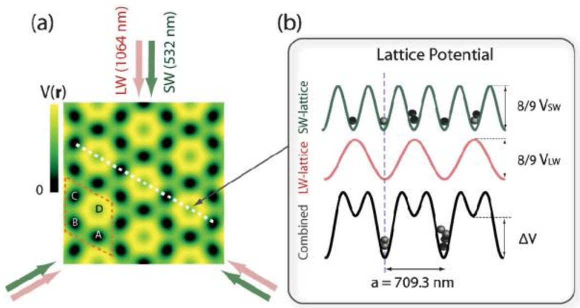


Triangular Lattice:



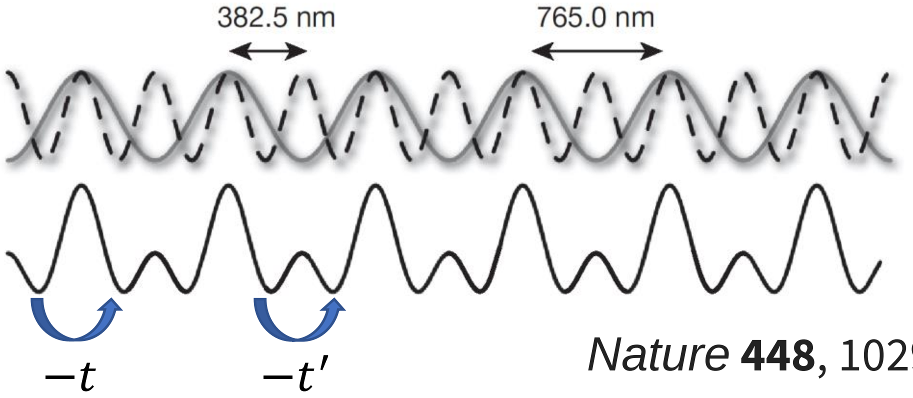
NJP 12 (2010) 065025

Kagome Lattice:



PRL 108, 045305 (2012)

Super Lattice:

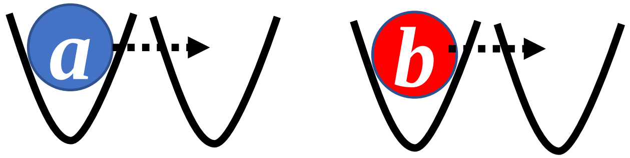


Nature **448**, 1029 (2007)

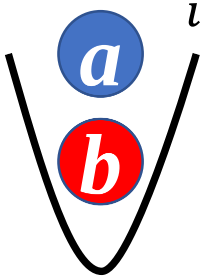
Multi-Component

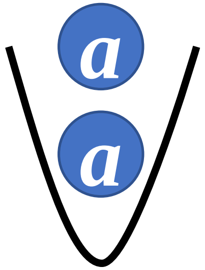
Two species Bose-Hubbard model:

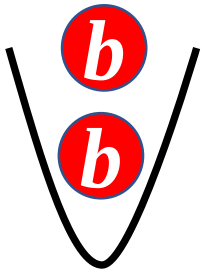
$$H = -t\sum_i \left(a_i^\dagger a_{i+1} + b_i^\dagger b_{i+1} + h.c.\right)$$

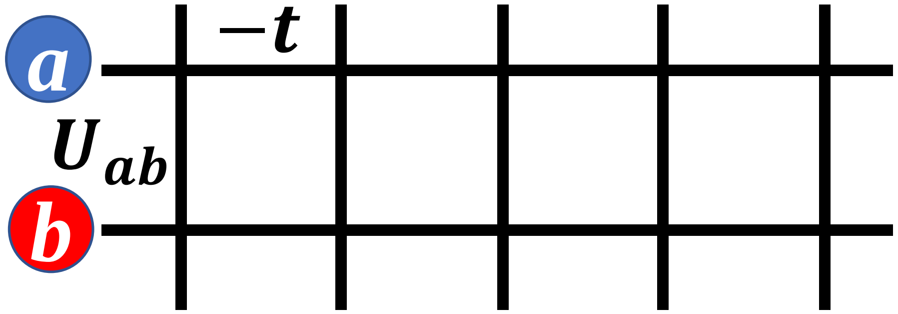


$$+U_{ab}\sum_i n_{ia}n_{ib} + U_{aa}\sum_i n_{ia}(n_{ia}-1) + U_{bb}\sum_i n_{ib}(n_{ib}-1)$$







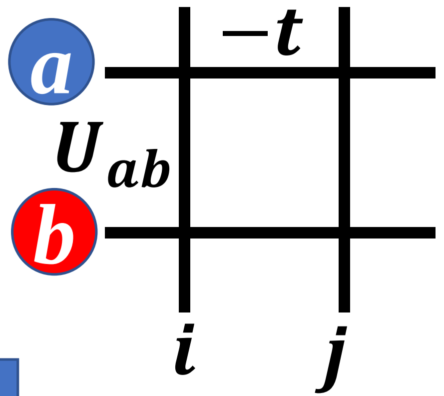


No hopping in vertical bonds !!!!

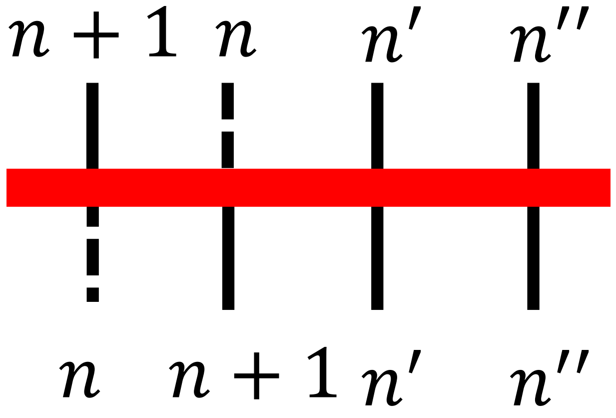
Cluster (Plaquette) SSE

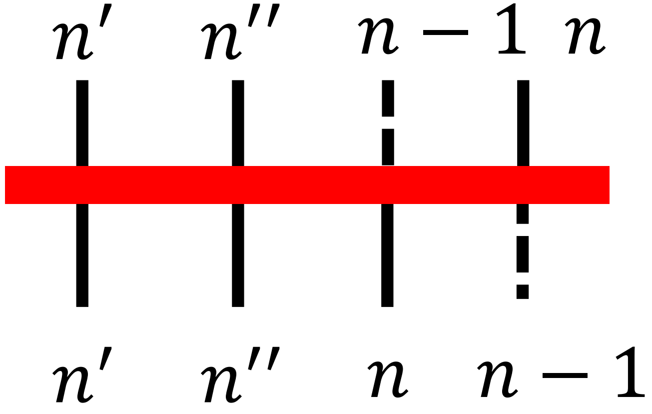
Hard-core limit: $U_{aa} \gg 1 \quad U_{bb} \gg 1$

Larger vertex:



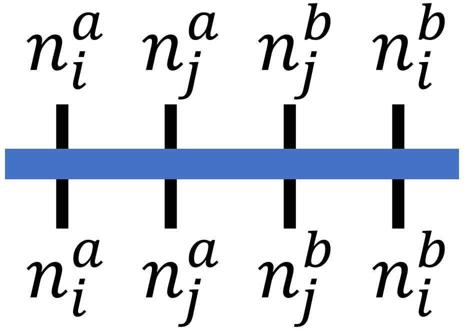
Off-Diagonal Operators:





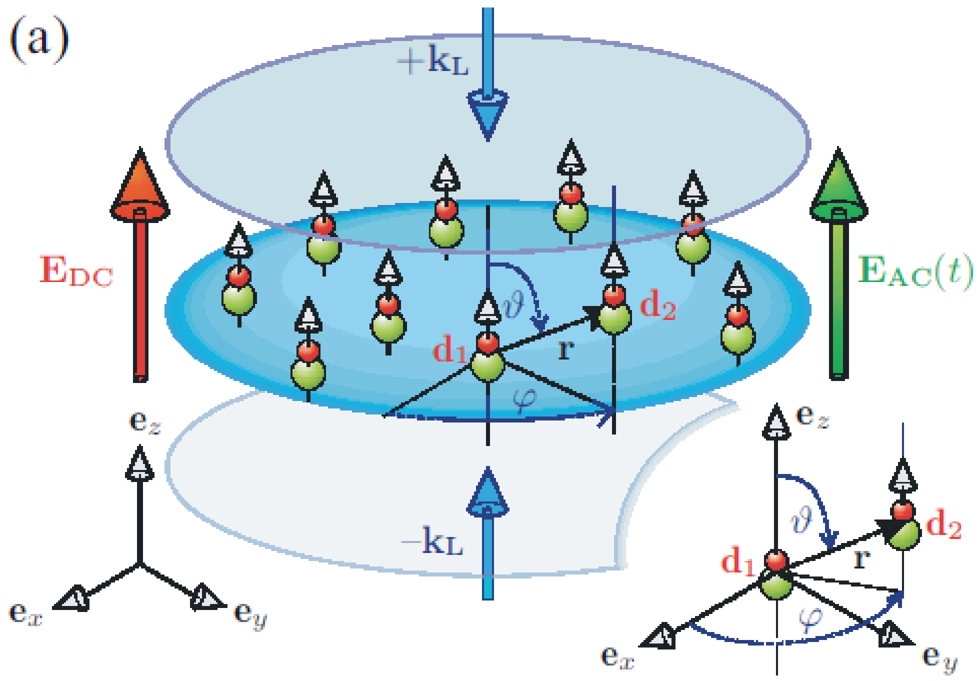
More updating choice!

Diagonal Operators:



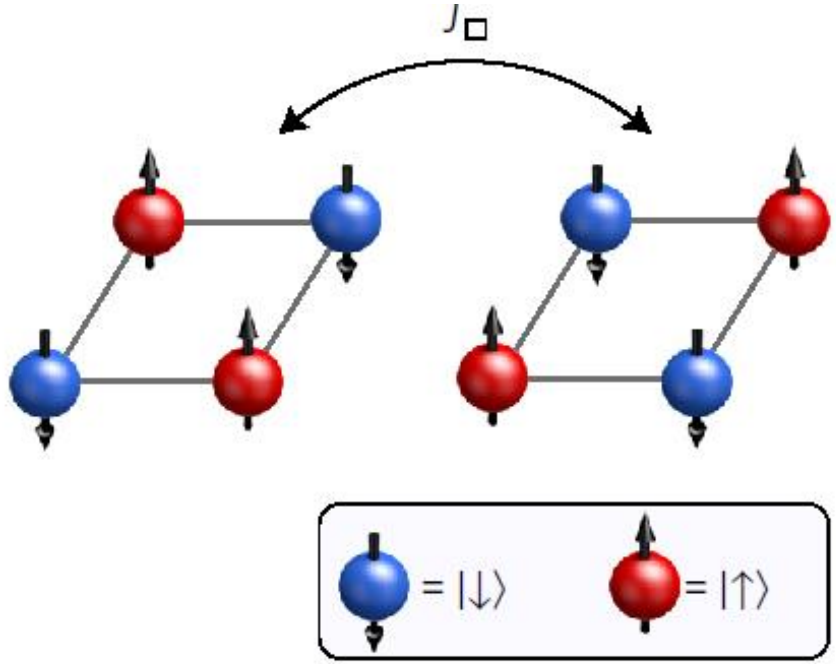
Many-body Interaction

Three body interaction:



Nature Physics **3**, 726 (2007)

Ring Exchange：



Nature Physics **13**, 1195 (2017)

Rydberg Array

Rydberg State

Rydberg state
(large principal
quantum number $n > 50$)

long lifetime (n^3):
$\sim 100\mu s$ @$n \approx 50$

Ground state

REVIEW ARTICLE
https://doi.org/10.1038/s41567-019-0733-z
nature physics

Many-body physics with individually controlled Rydberg atoms

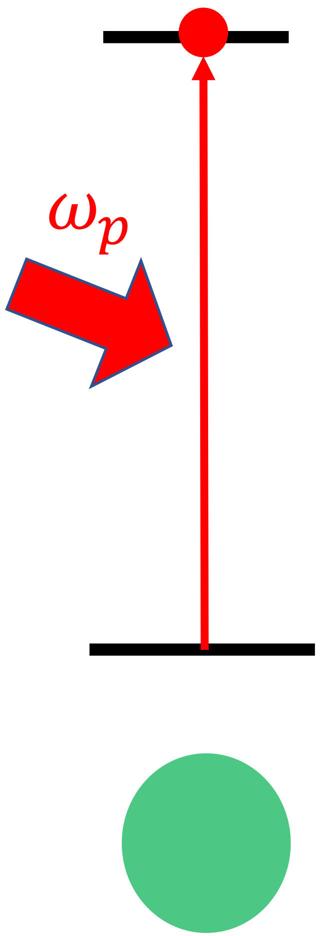
Antoine Browaeys * and Thierry Lahaye

Two-Level ensembles:

$|e\rangle$: Rydberg state

$|g\rangle$: Ground state

Rydberg State



Rydberg state (large principal quantum number $n > 50$)

long lifetime (n^3):

$\sim 100\mu s\ @n \approx 50$

Ground state

REVIEW ARTICLE
https://doi.org/10.1038/s41567-019-0733-z
nature physics

Many-body physics with individually controlled Rydberg atoms

Antoine Browaeys* and Thierry Lahaye

Two-Level ensembles:

$|e\rangle$: Rydberg state

$|g\rangle$: Ground state

Rabi model:

Detuning : $\delta = (\omega_c - \omega_p)$

$$H = \frac{\hbar}{2}(\omega_c - \omega_p)|e\rangle\langle e| + \frac{\hbar\Omega}{2}(|e\rangle\langle g| + h.c.)$$

Energy gap: $\hbar\omega_c$ Laser frequency: ω_p

Rabi frequency: Ω (proportional to laser power)

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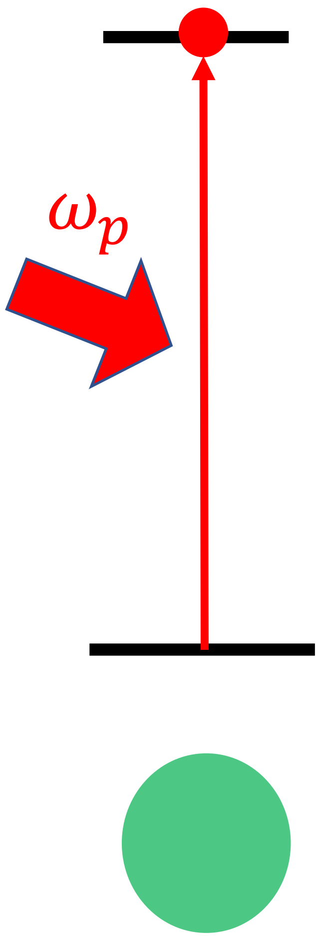
Rydberg State



Rydberg state
(large principal
quantum number $n > 50$)

long lifetime (n^3):
$\sim 100\mu s$ @$n \approx 50$

Ground state

Preparing random states and benchmarking with many-body quantum chaos

Joonhee Choi, Adam L. Shaw, Ivaylo S. Madjarov, Xin Xie, Ran Finkelstein, Jacob P. Covey, Jordan S. Cotler, Daniel K. Mark, Hsin-Yuan Huang, Anant Kale, Hannes Pichler, Fernando G. S. L. Brandão, Soonwon Choi & Manuel Endres

Nature **613**, 468–473 (2023) | Cite this article

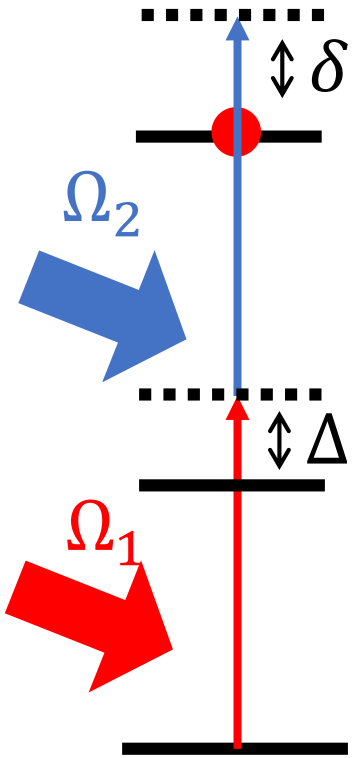
Sr-88 atoms:

$|e\rangle$: $5s61s\,{}^3S_1, m_J = 0$

$|g\rangle$: $5s5p\,{}^3P_0$ $(clock\ state)$

UV laser: $\omega_c = 317nm$

Two-photon process



Rydberg state $|e\rangle$
(large principal quantum number $n > 50$)

Intermediate state $|i\rangle$

Ground state $|g\rangle$

LETTER
doi:10.1038/nature11596

Observation of spatially ordered structures in a two-dimensional Rydberg gas

Peter Schauß[1], Marc Cheneau[1], Manuel Endres[1], Takeshi Fukuhara[1], Sebastian Hild[1], Ahmed Omran[1], Thomas Pohl[2], Christian Gross[1], Stefan Kuhr[1,3] & Immanuel Bloch[1,4]

Rb-87 atoms:

$|e\rangle$ $|43S_{1/2}, m_J = -1/2\rangle$

$|i\rangle$ $|5P_{3/2}, F = 3, m_J = -3\rangle$

$|g\rangle$ $|5S_{1/2}, F = 2, m_J = -2\rangle$

$\omega_1 = 780nm$ $\omega_2 = 480nm$

$$\Omega = \frac{\Omega_1 \Omega_2}{2\Delta}$$

Adiabatic Elimination
Large Δ

Dipole-dipole Interaction

Strong long range interaction:

$$V_{EDDI} = \frac{C_3}{R^3} \longrightarrow V_{vdw} = \frac{C_6}{R^6}$$

$$C_6 \propto n^{11}$$

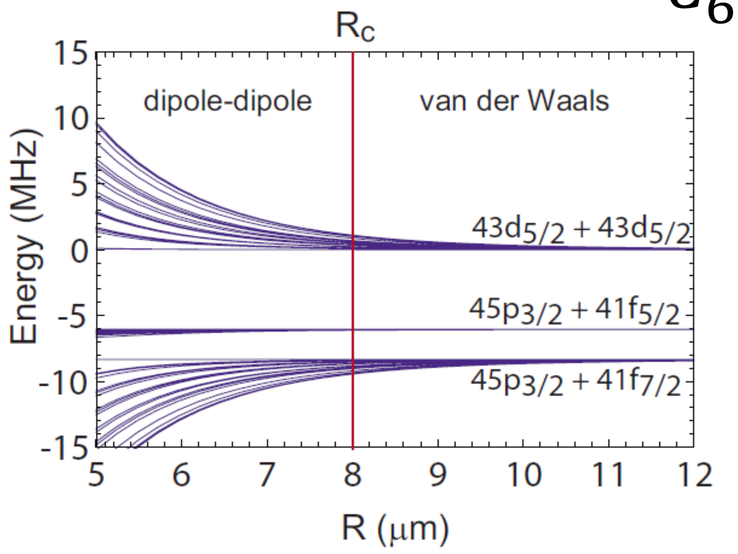
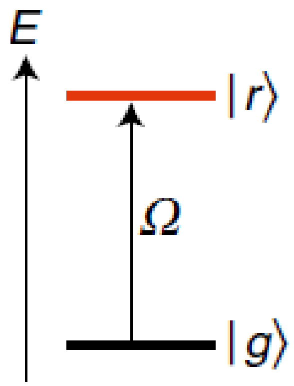
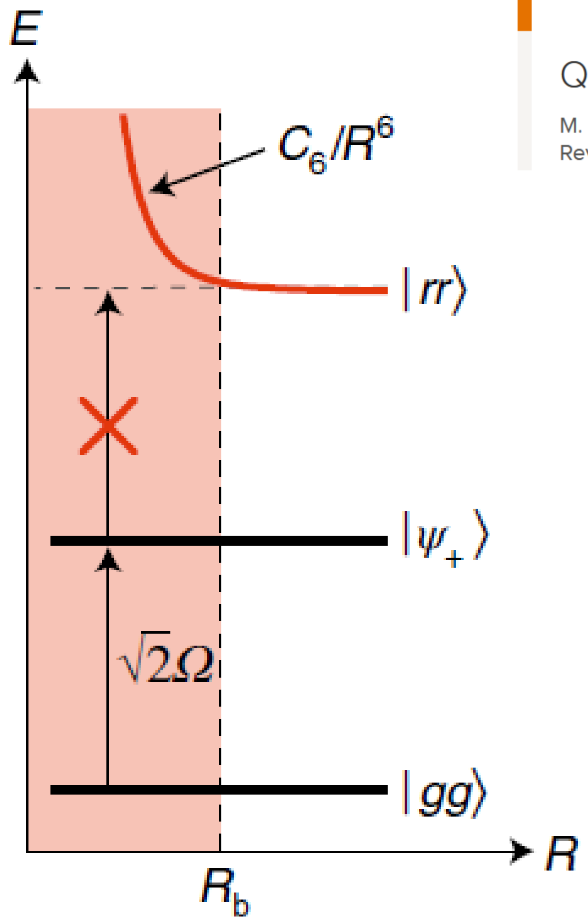


FIG. 9. (Color online) Interaction potentials for $43d_{5/2} + 43d_{5/2}$ Rb Rydberg atoms. The cutoff radius R_c represents the distance scale for the transition from resonant dipole-dipole to van der Waals behavior.





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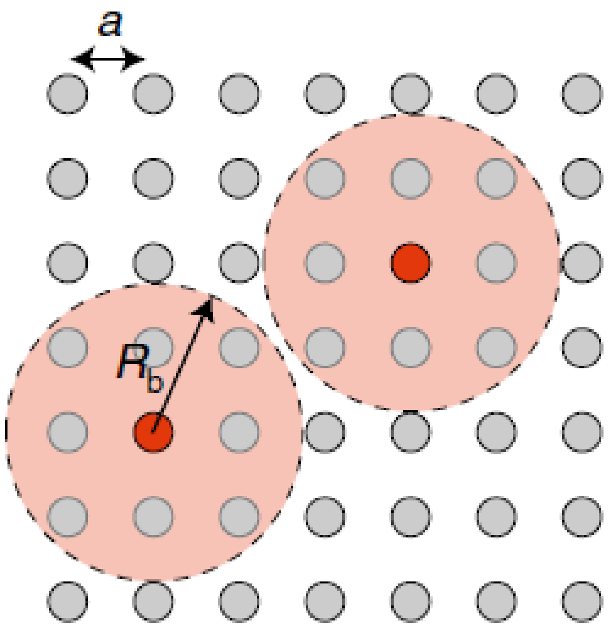
Quantum information with Rydberg atoms

M. Saffman, T. G. Walker, and K. Mølmer

Rev. Mod. Phys. **82**, 2313 – Published 18 August 2010



Dipole-dipole Interaction

Quantum Many body Hamiltonian:

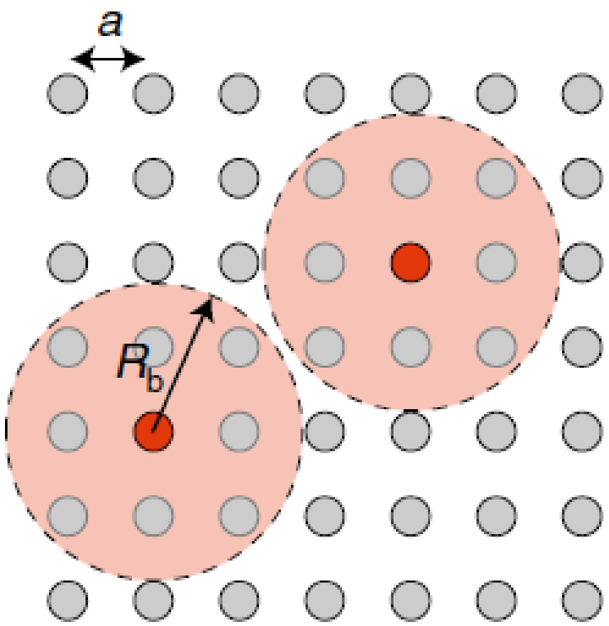
$$H = \frac{\hbar}{2}\delta\sum_i n_i + \frac{\hbar\Omega}{2}\sum_i \sigma_i^x + \sum_{i,j} V_{ij} n_i n_j$$

$$V_{ij} = \frac{C_6}{(R_i - R_j)^6}$$

$$n = |e\rangle\langle e| = \frac{\sigma^z + 1}{2} \qquad \sigma^x = |e\rangle\langle g| + |g\rangle\langle e|$$

Blockade radius:

$\hbar\Omega \ll C_6/R_b^6$ → $R_b = \left(\frac{C_6}{\hbar\Omega}\right)^{1/6} \sim 5\mu m$



Rydberg atom in optical lattice

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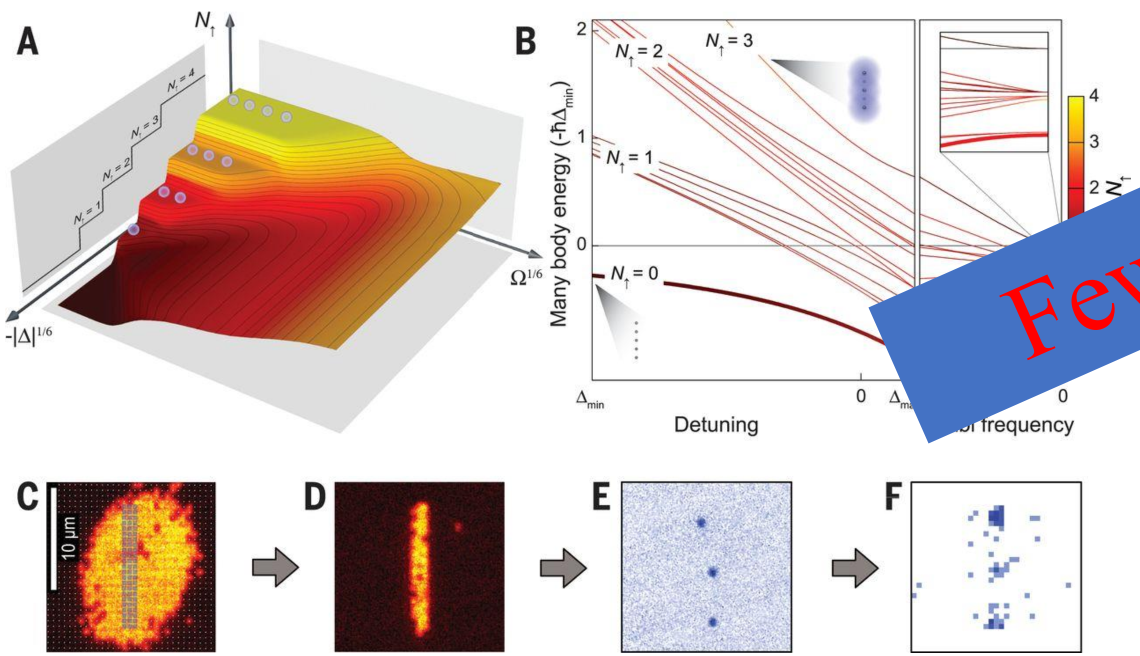
HOME > SCIENCE > VOL. 347, NO. 6229 > CRYSTALLIZATION IN ISING QUANTUM MAGNETS

Crystallization in Ising quantum magnets

P. SCHAUSS , J. ZEIHER, T. FUKUHARA, S. HILD, M. CHENEAU, T. MACRÌ, T. POHL, I. BLOCH, AND C. GROSS Authors Info & Affiliations

SCIENCE • 27 Mar 2015 • Vol 347, Issue 6229 • pp. 1455-1458 • DOI: 10.1126/science.1258351



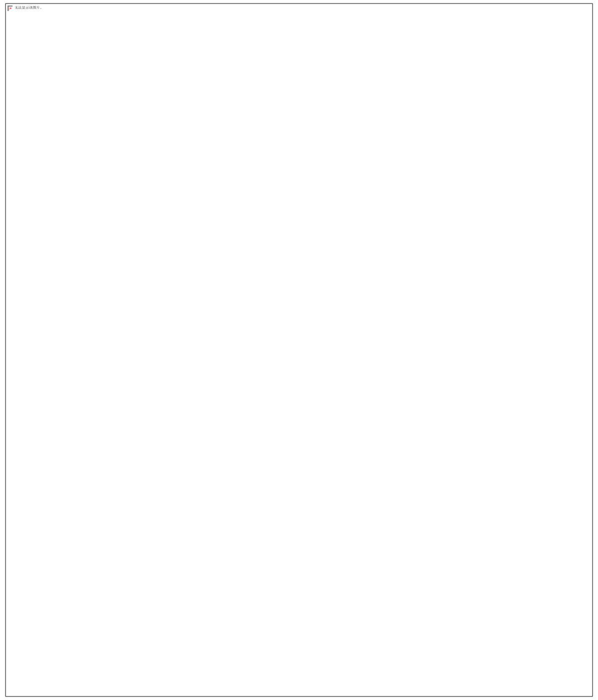
Published: 31 October 2012

Observation of spatially ordered structures in a two-dimensional Rydberg gas

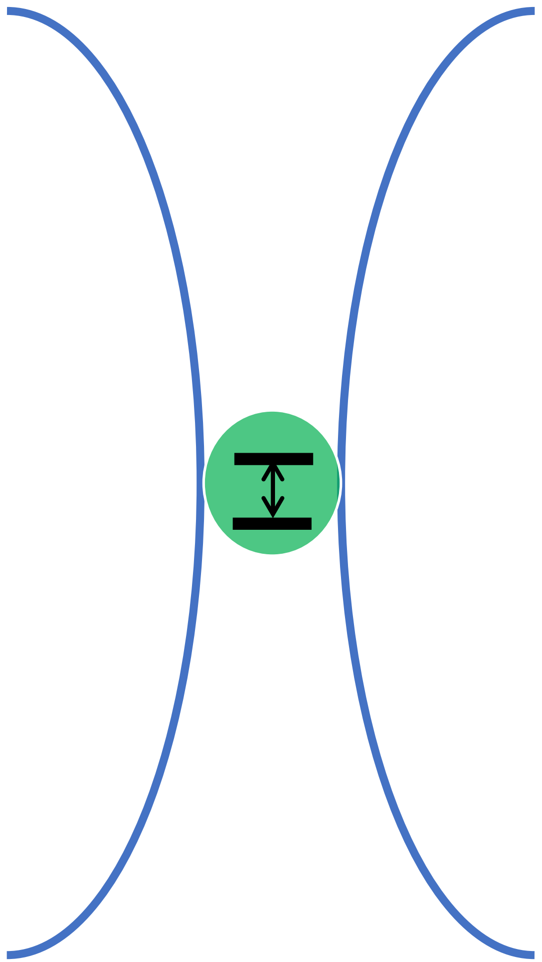
Peter Schauß, Marc Cheneau, Manuel Endres, Takeshi Fukuhara, Sebastian Hild, Ahmed Omran, Thomas Pohl, Christian Gross, Stefan Kuhr & Immanuel Bloch

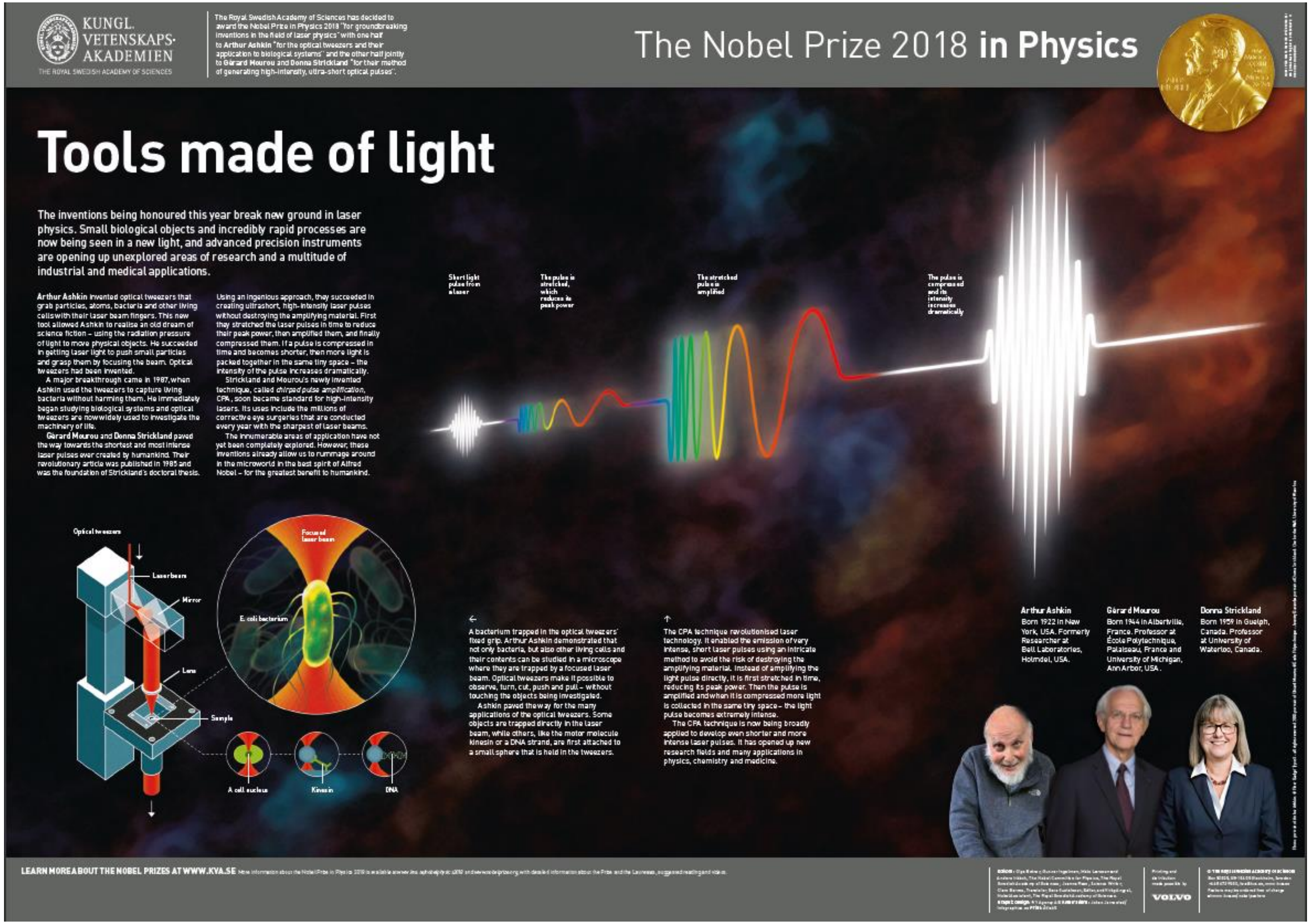
Nature **491**, 87–91 (2012) | Cite this article

Few atoms !!!



Optical Tweezer





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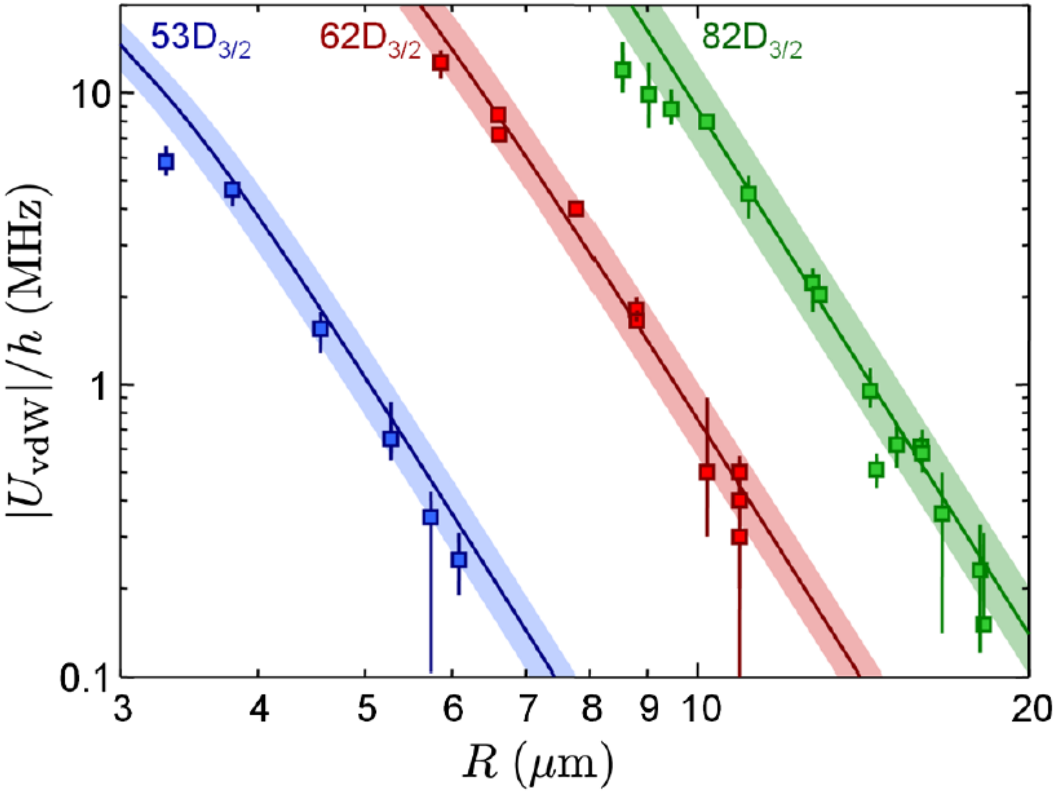
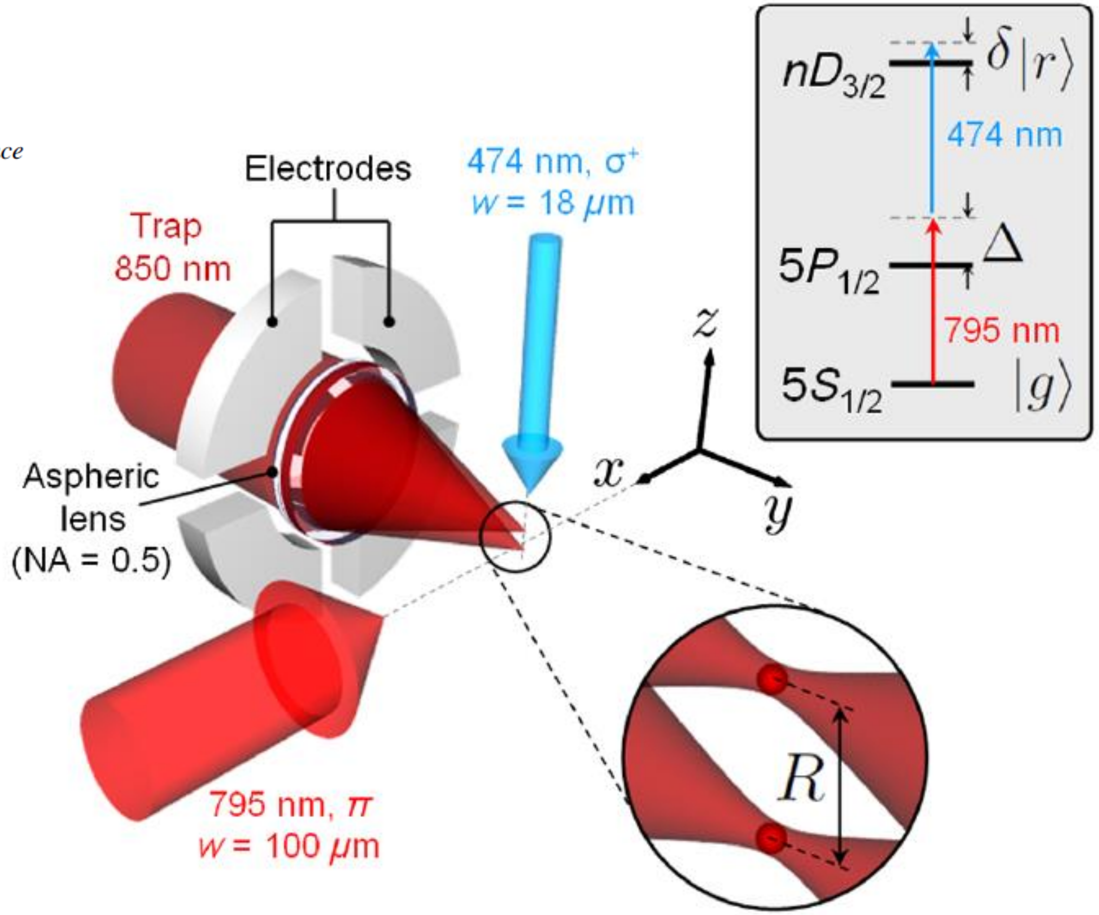
Optical Tweezer

Selected for a Viewpoint in *Physics*
PRL **110**, 263201 (2013) PHYSICAL REVIEW LETTERS week ending 28 JUNE 2013

Direct Measurement of the van der Waals Interaction between Two Rydberg Atoms

L. Béguin,[1] A. Vernier,[1] R. Chicireanu,[2] T. Lahaye,[1] and A. Browaeys[1]
[1]*Laboratoire Charles Fabry, Institut d'Optique, CNRS, Univ Paris Sud, 2 avenue Augustin Fresnel, 91127 Palaiseau cedex, France*
[2]*Laboratoire de Physique des Lasers, Atomes et Molécules, Université Lille 1, CNRS; 59655 Villeneuve d'Ascq cedex, France*
(Received 22 March 2013; published 24 June 2013)





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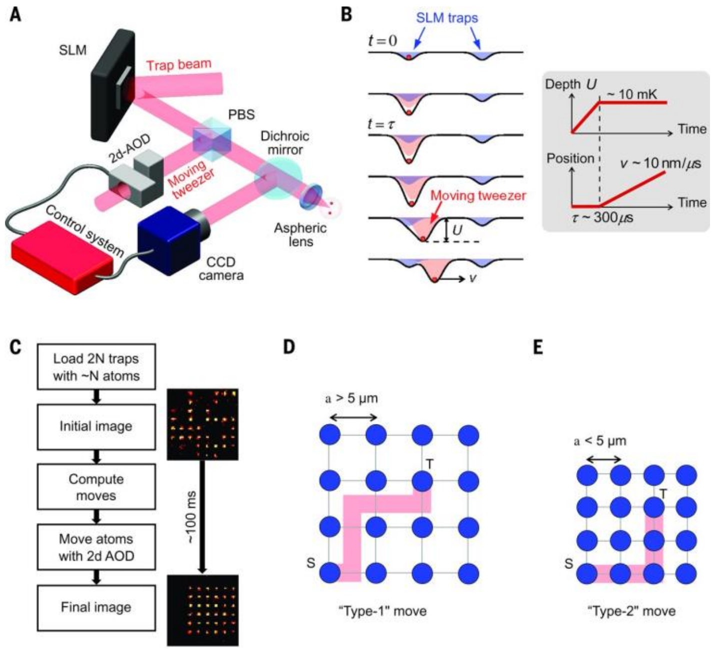
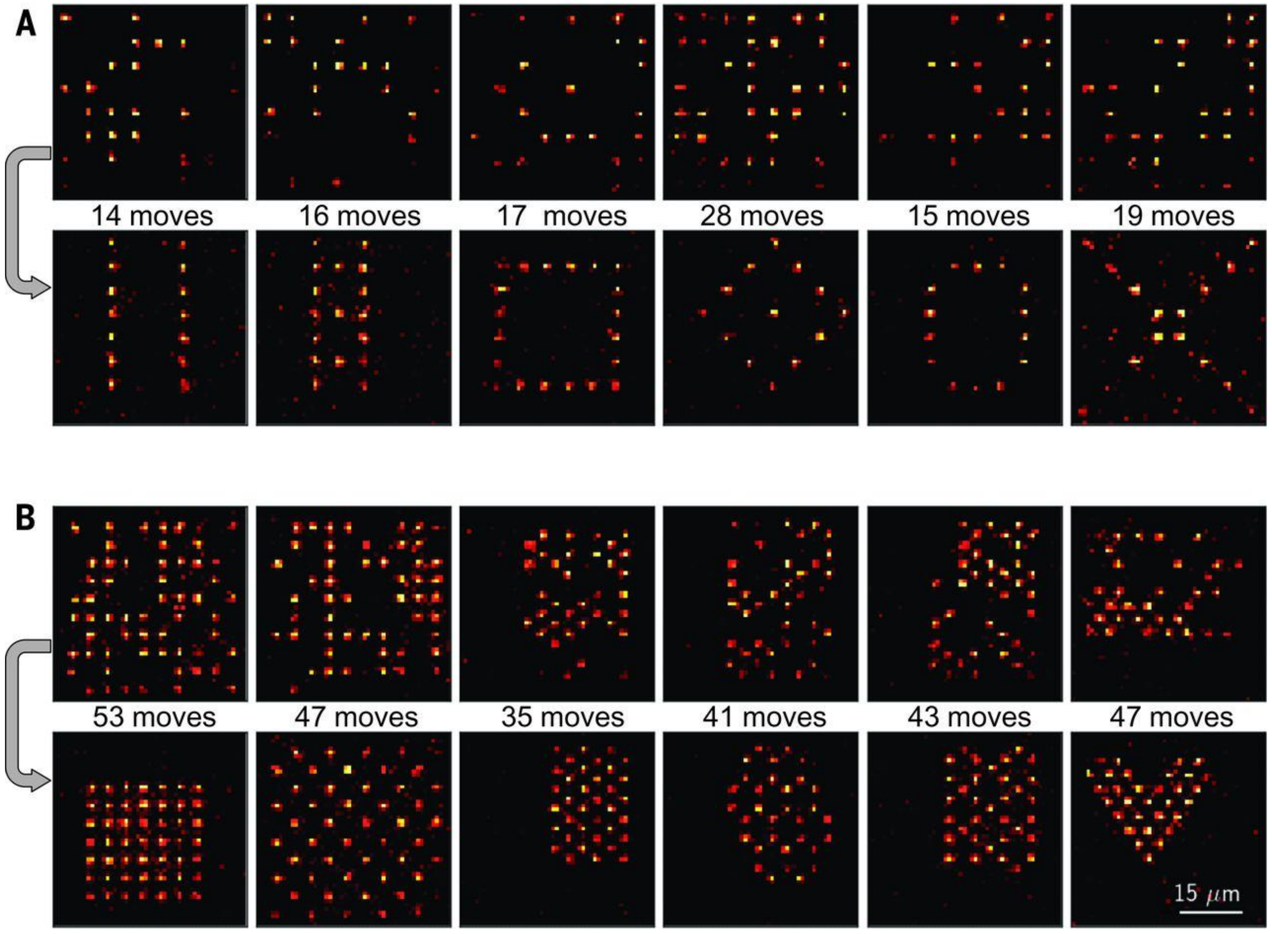
REPORT

An atom-by-atom assembler of defect-free arbitrary two-dimensional atomic arrays

DANIEL BARREDO, SYLVAIN DE LÉSÉLEUC, VINCENT LIENHARD, THIERRY LAHAYE , AND ANTOINE BROWAEYS Authors Info & Affiliations

SCIENCE • 3 Nov 2016 • Vol 354, Issue 6315 • pp. 1021-1023 • DOI: 10.1126/science.aah3778





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Letter | Published: 05 September 2018

Synthetic three-dimensional atomic structures assembled atom by atom

Daniel Barredo, Vincent Lienhard, Sylvain de Léséleuc, Thierry Lahaye & Antoine Browaeys

Nature **561**, 79–82 (2018) | Cite this article

Rydberg Array

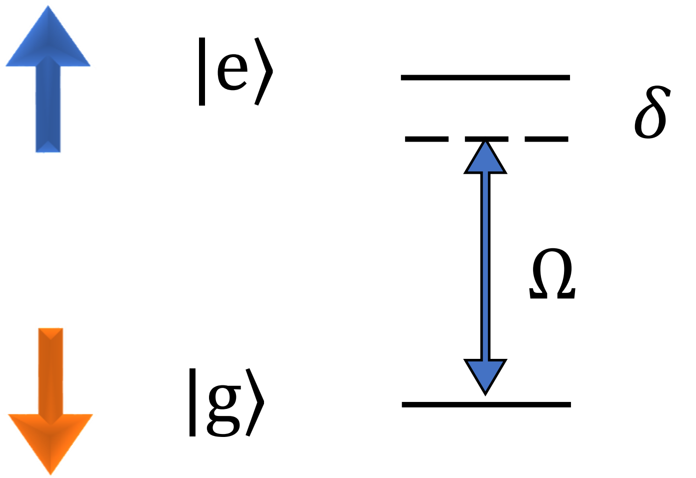
Article

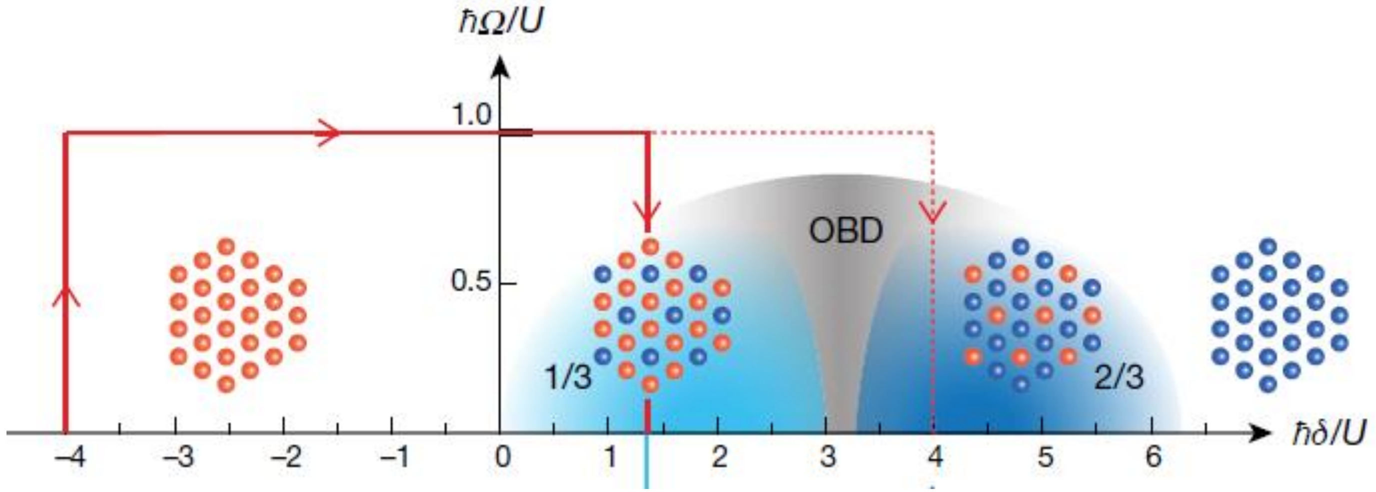
Quantum simulation of 2D antiferromagnets with hundreds of Rydberg atoms

https://doi.org/10.1038/s41586-021-03585-1

Received: 21 December 2020

Pascal Scholl[1,6] ✉, Michael Schuler[2,6], Hannah J. Williams[1,6], Alexander A. Eberharter[3,6], Daniel Barredo[1,4], Kai-Niklas Schymik[1], Vincent Lienhard[1], Louis-Paul Henry[5], Thomas C. Lang[3], Thierry Lahaye[1], Andreas M. Läuchli[3] & Antoine Browaeys[1]





Pascal Scholl, et. al Nature **595**, 233 (2021)

$$H=\sum_{ij}\frac{C_6}{r_{ij}^6}n_i n_j-\frac{\Omega}{2}\sum_i\sigma_i^x+\frac{\delta}{2}\sum_i\sigma_i^z$$

$n_i \rightarrow (S_i^Z+1)/2$

$$H=\sum_{ij}J_{ij}S_i^Z S_j^Z-\Omega\sum_i S_i^x+\delta\sum_i S_i^z$$

SLM | Laser power | Laser frequency

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Trapped Ion

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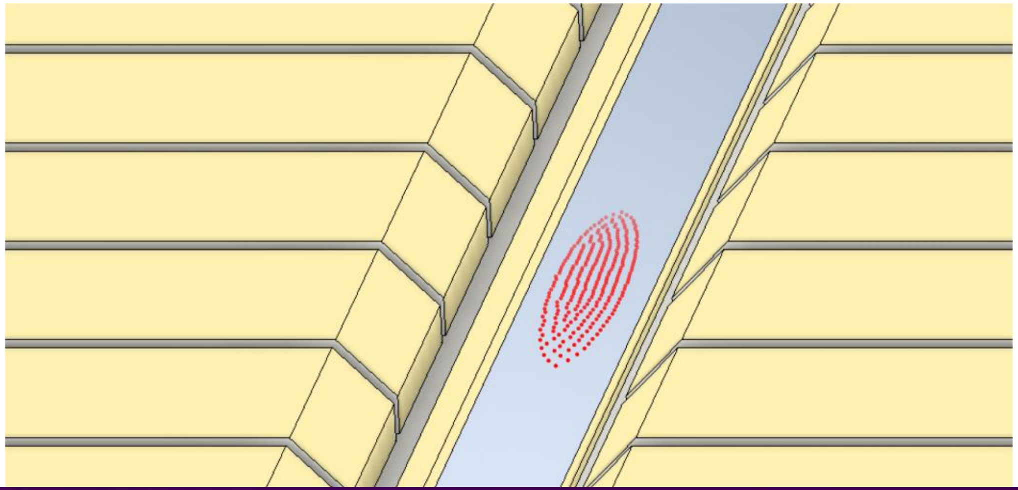
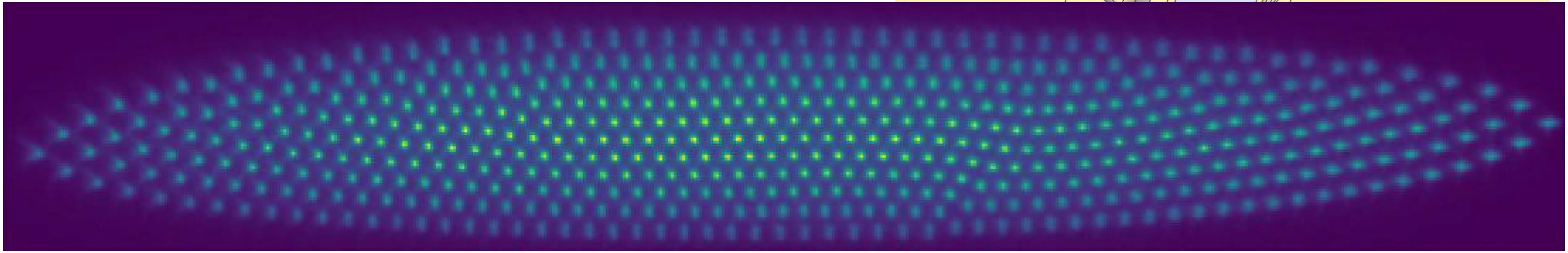
Article | Published: 29 May 2024

A site-resolved two-dimensional quantum simulator with hundreds of trapped ions

S.-A. Guo, Y.-K. Wu, J. Ye, L. Zhang, W.-Q. Lian, R. Yao, Y. Wang, R.-Y. Yan, Y.-J. Yi, Y.-L. Xu, B.-W. Li, Y.-H. Hou, Y.-Z. Xu, W.-X. Guo, C. Zhang, B.-X. Qi, Z.-C. Zhou, L. He & L.-M. Duan

$$H = \sum_{ij} J_{ij} S_i^Z S_j^Z - \Omega \sum_i S_i^x + \delta \sum_i S_i^z$$





D-Wave

Letter | Published: 22 August 2018

Observation of topological phenomena in a programmable lattice of 1,800 qubits

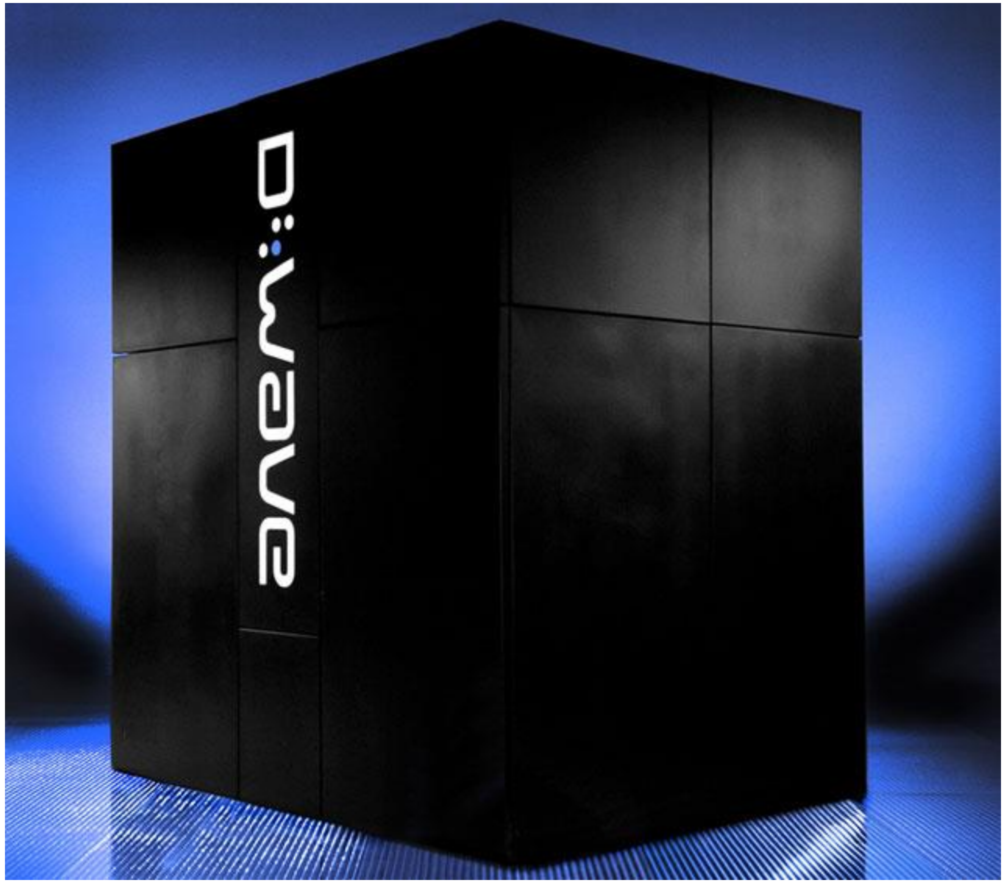
Andrew D. King, Juan Carrasquilla, Jack Raymond, Isil Ozfidan, Evgeny Andriyash, Andrew Berkley, Mauricio Reis, Trevor Lanting, Richard Harris, Fabio Altomare, Kelly Boothby, Paul I. Bunyk, Colin Enderud, Alexandre Fréchette, Emile Hoskinson, Nicolas Ladizinsky, Travis Oh, Gabriel Poulin-Lamarre, Christopher Rich, Yuki Sato, Anatoly Yu. Smirnov, Loren J. Swenson, Mark H. Volkmann, Jed Whittaker, ... Mohammad H. Amin + Show authors

Nature **560**, 456–460 (2018) | Cite this article

value for near-term quantum computing technologies[14,15]. Quantum annealing (QA) processors[16–18] can be used to simulate systems in the transverse-field Ising model (TFIM) described by the Hamiltonian

$$H = \sum_i h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x \qquad (1)$$

where h_i are longitudinal fields, J_{ij} are coupling terms, σ_i^x and σ_i^z are Pauli matrices acting on the ith spin, and Γ is the transverse field.



SSE for Rydberg Array

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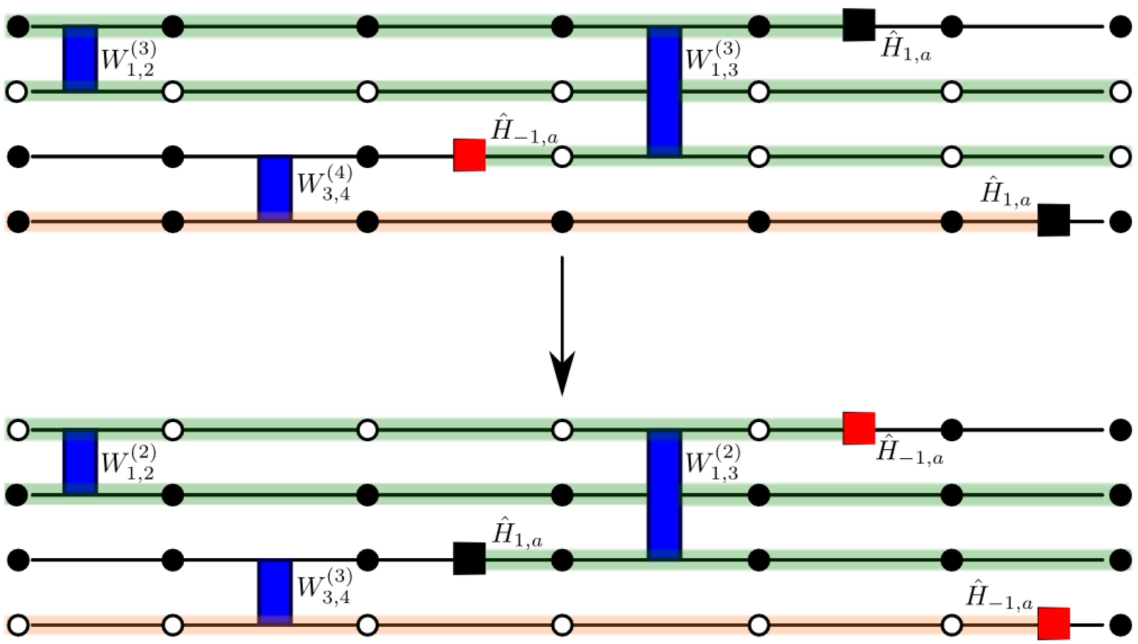
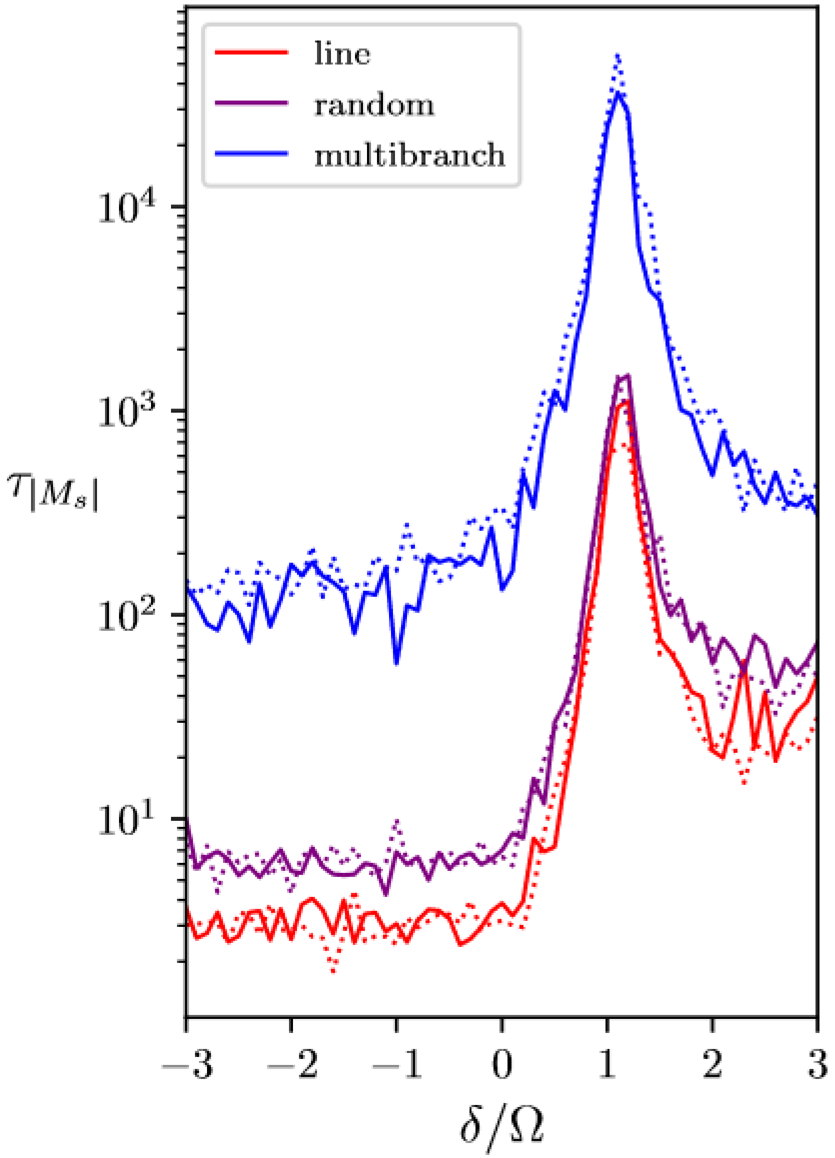
Stochastic series expansion quantum Monte Carlo for Rydberg arrays

Ejaaz Merali, Isaac J. S. De Vlugt, Roger G. Melko

SciPost Phys. Core 7, 016 (2024) · published 5 April 2024





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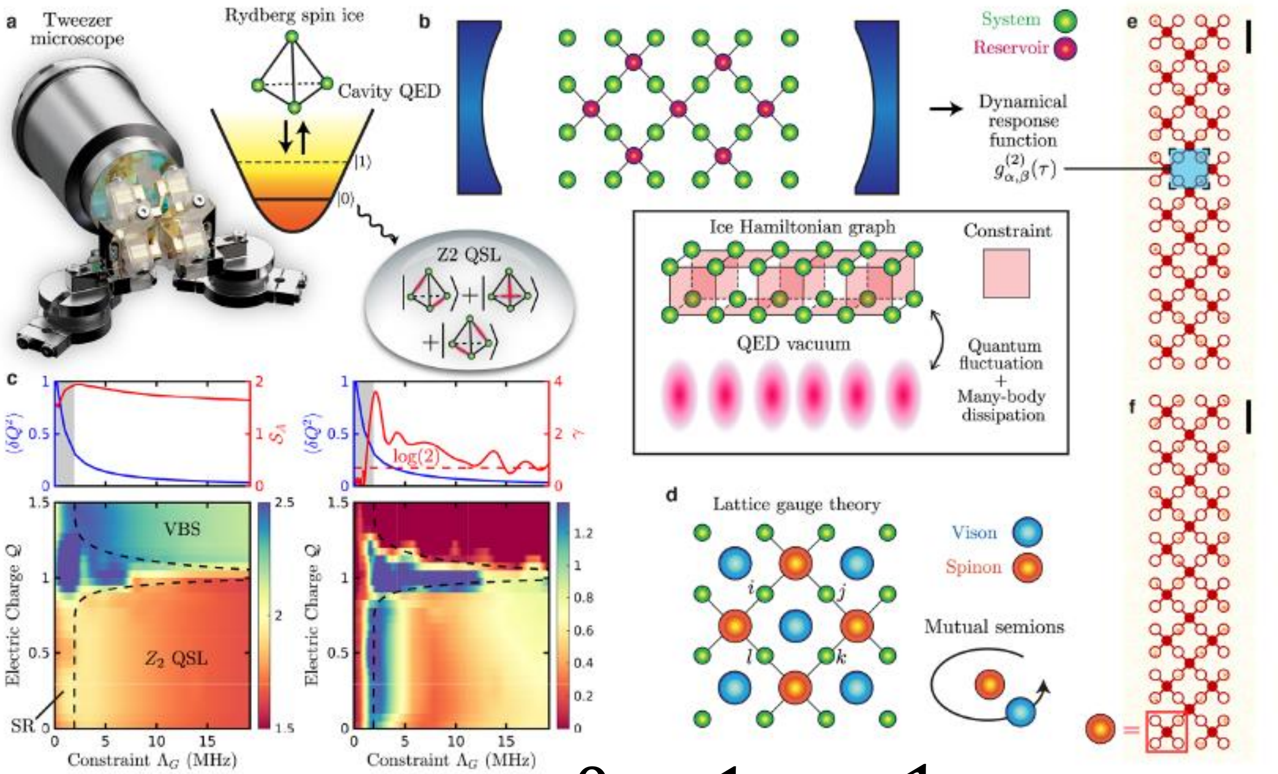
Rydberg Array in a Cavity?

Melting a Rydberg ice to a topological spin liquid with cavity vacuum fluctuation

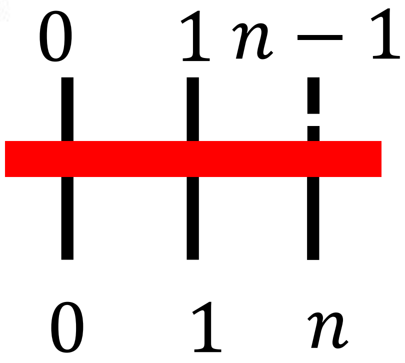
H. R. Kong, J. Taylor, Y. Dong, K. S. Choi

Quantum spin liquids are exotic phases of matter that are prevented from being frozen even at zero temperature, and appear disordere by local probes that monitor the subsystems. Driven by quantum fluctuations, topological spin liquids are manifested by their long-range entanglement, and are characterized by quasiparticles with fractional statistics. Here, we make contact of a 2D Rydberg ice to a QED vacuum of an ultra-high-finesse optical cavity, and dynamically promote the frustrated background field of the spin ice to a $\mathbb{Z}_2$ spin liquic We characterize the deconfined nature of the dynamical gauge theory residing in the strongly-correlated Rydberg matter with Wilsonian loops. We observe the proliferation of vison and spinon pairs by site-resolved fluorescence imaging, and detect the exchange statistical angle $\theta_{top} \sim \pi/2$ between the two anyons by monitoring the dynamical correlators of the fluctuating cavity photons. Our work provides the first microscopic detection of anyons in a topological quantum matter, and heralds the arrival of strongly-coupled many-body QED, where interacting matter and light are put on equal footing at the level of individual quanta.

Comments: This preprint is withdrawn due to incorrect result
Subjects: **Quantum Physics (quant-ph)**; Quantum Gases (cond-mat.quant-gas); Atomic Physics (physics.atom-ph)
Cite as: arXiv:2109.03741 **[quant-ph]**



$$H = \sum_{ij} \frac{C_6}{r_{ij}^6} n_i n_j - g \sum_i \sigma_i^x (a^\dagger + a) + \frac{\delta}{2} \sum_i \sigma_i^z + \omega a^\dagger a$$



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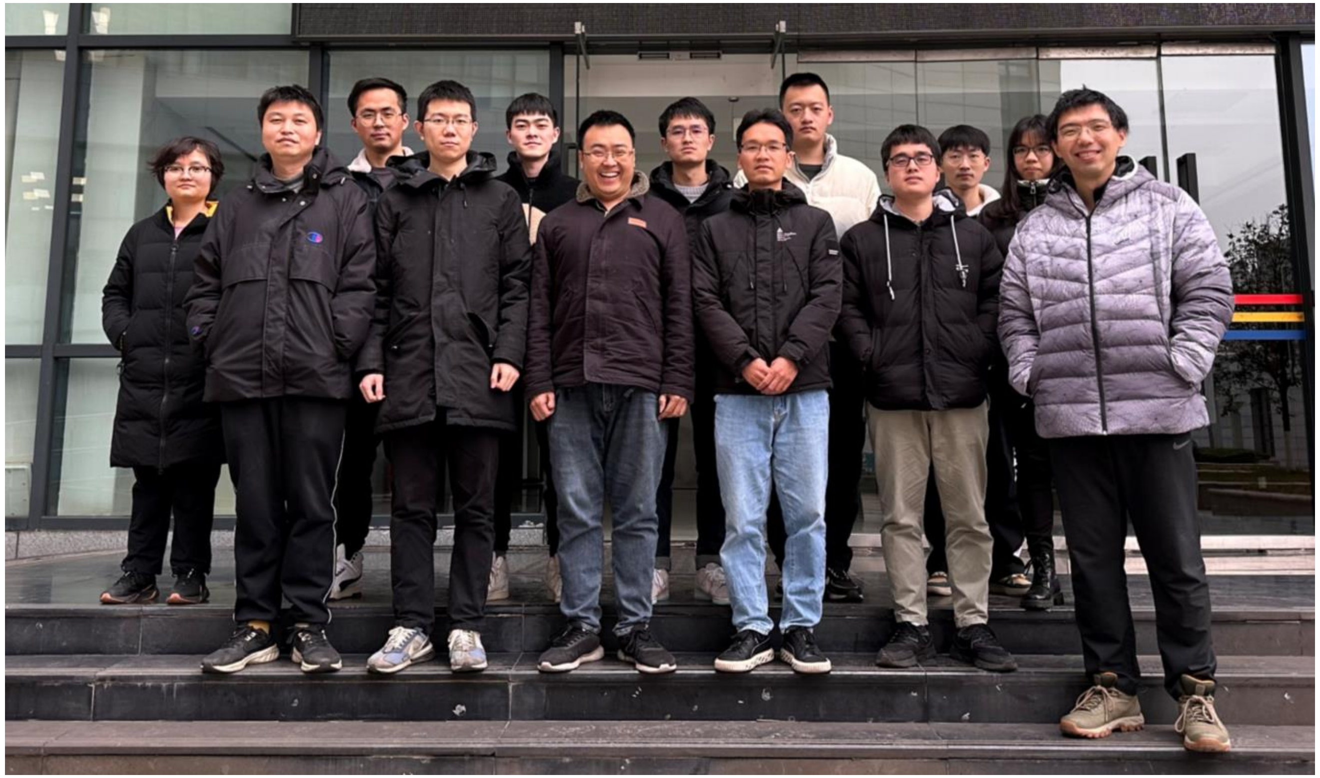

Zheng Yan
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Yan-Cheng Wang
(BAAU)

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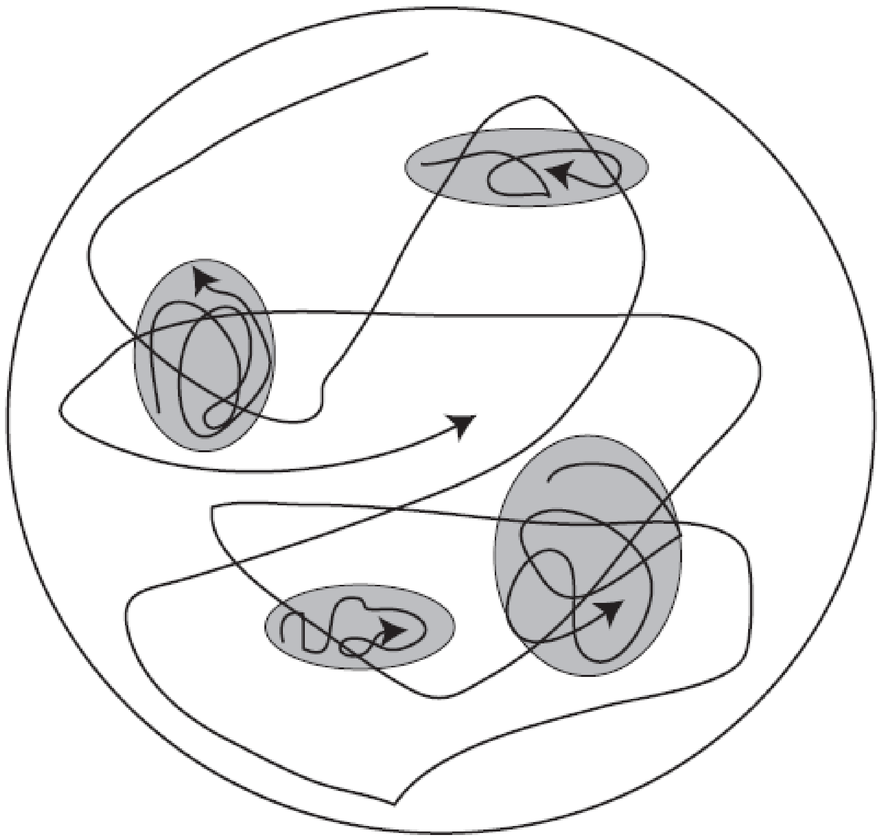
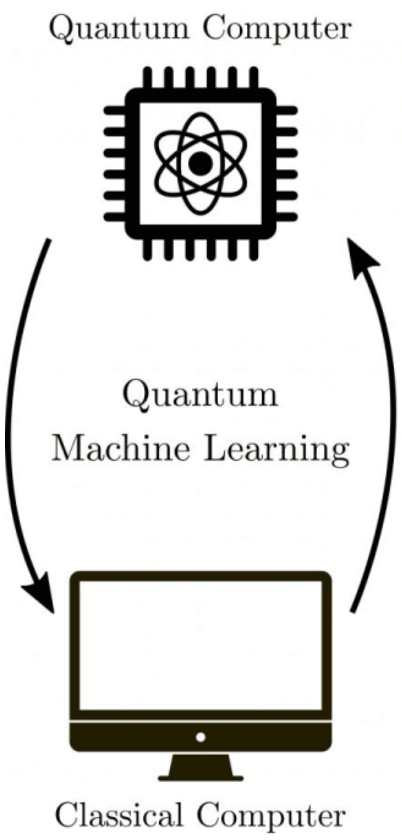
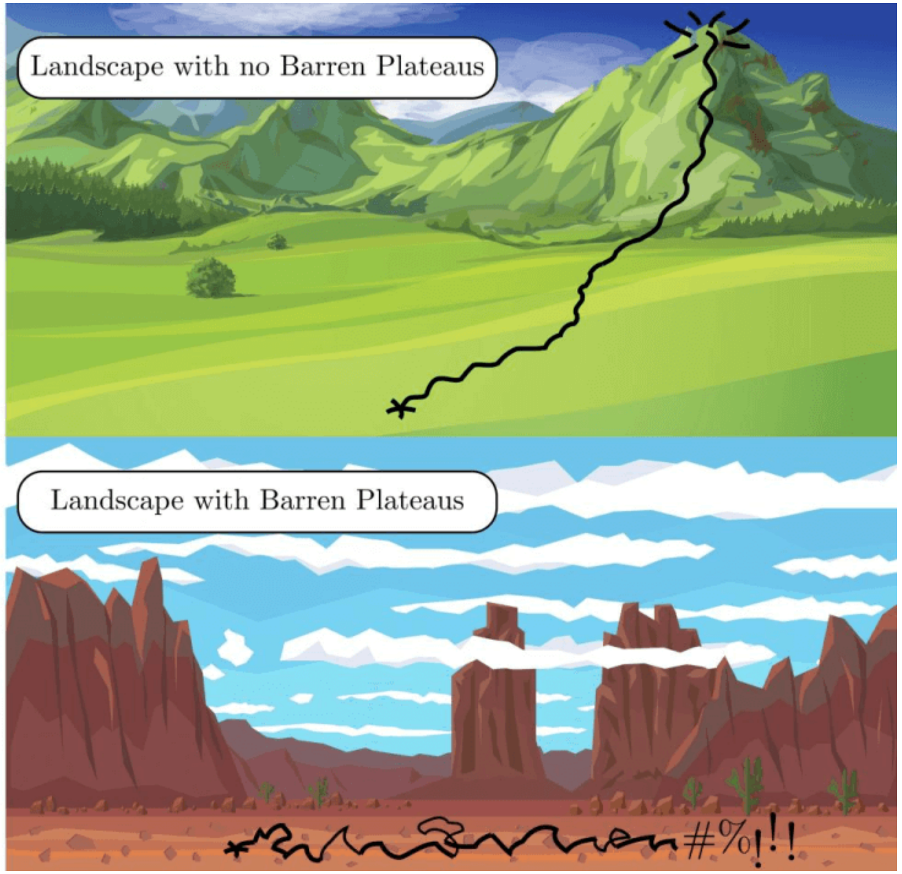
Parallel Tempering

Why we need the Parallel Tempering:



Barren Plateaus:





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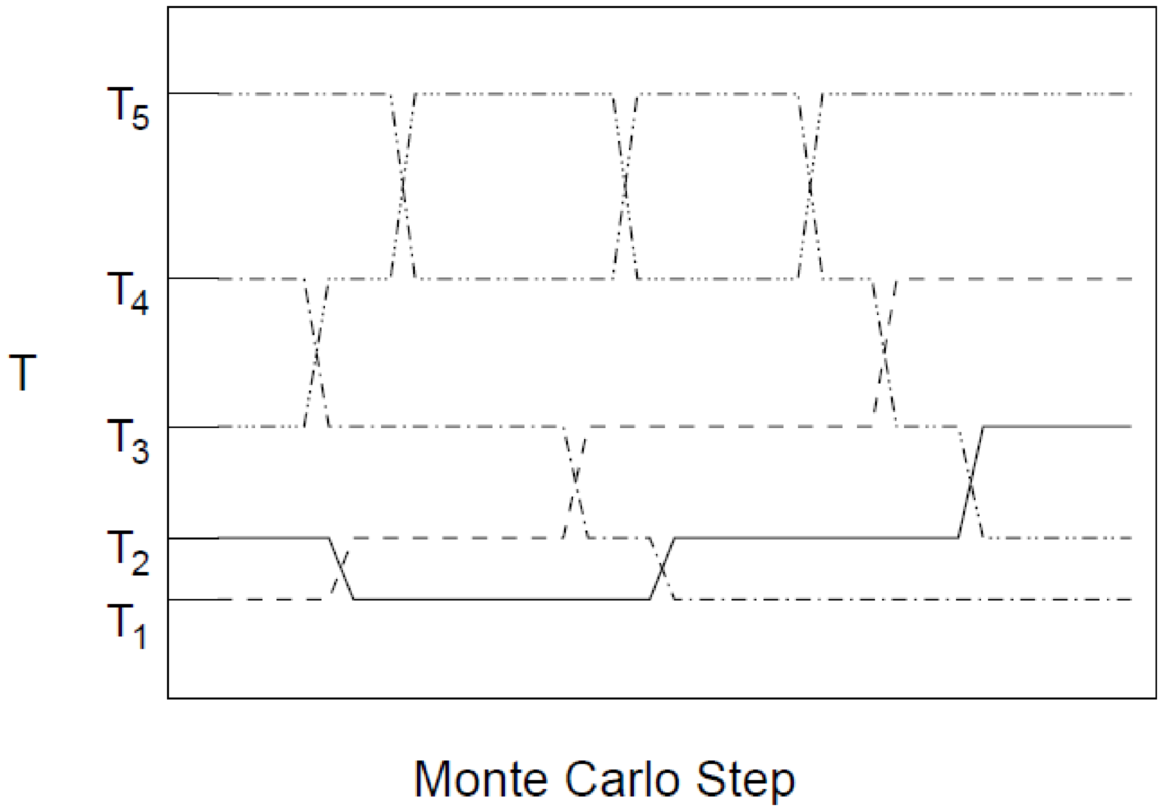
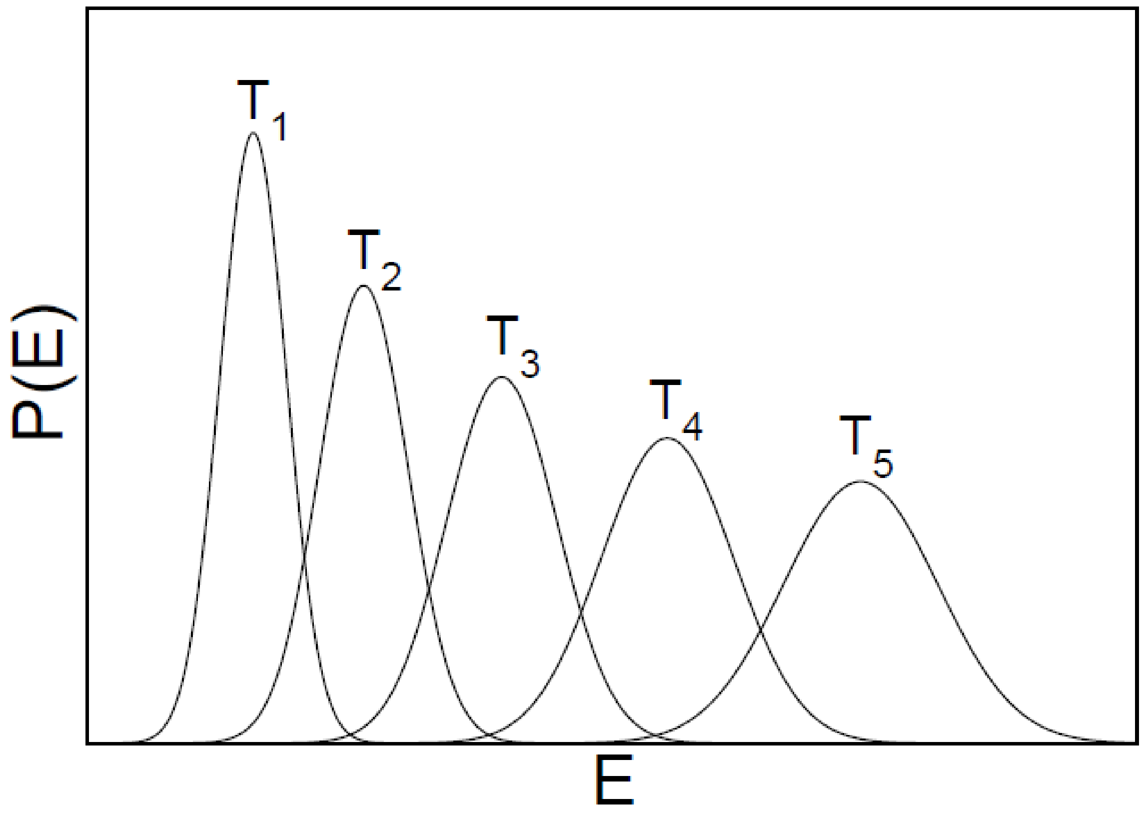
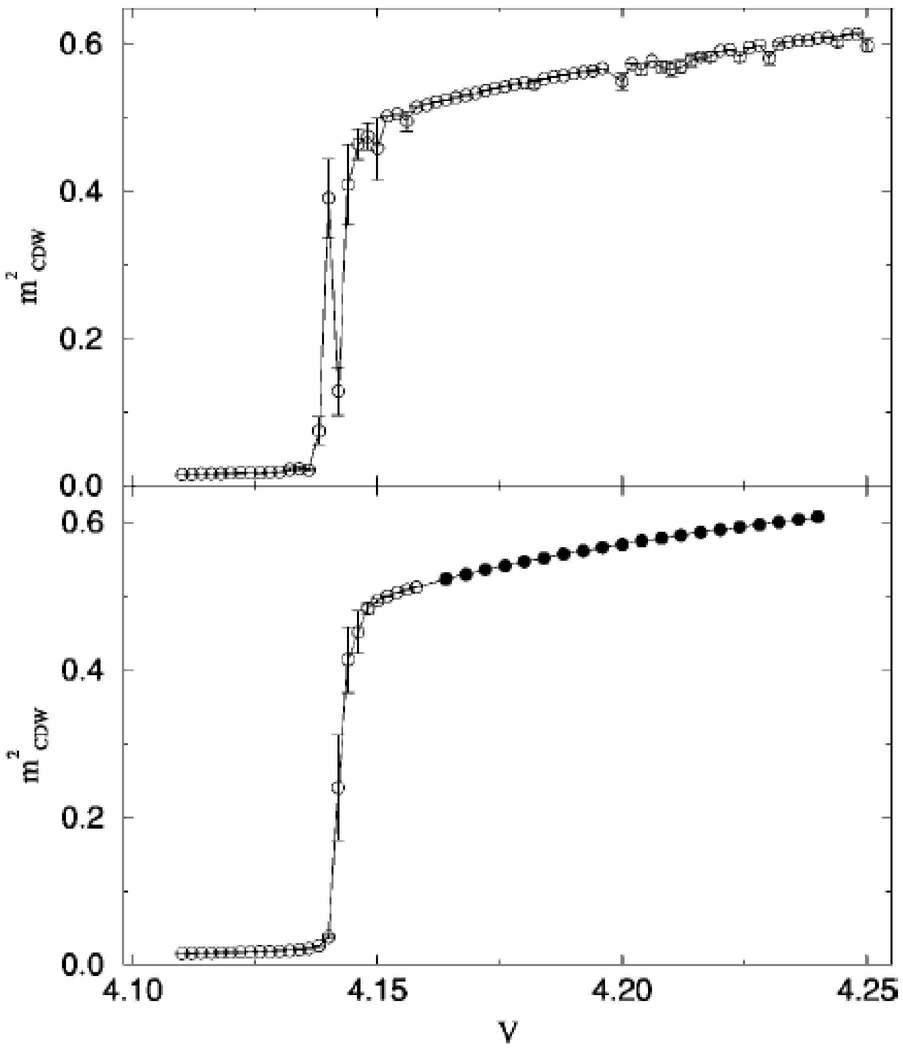
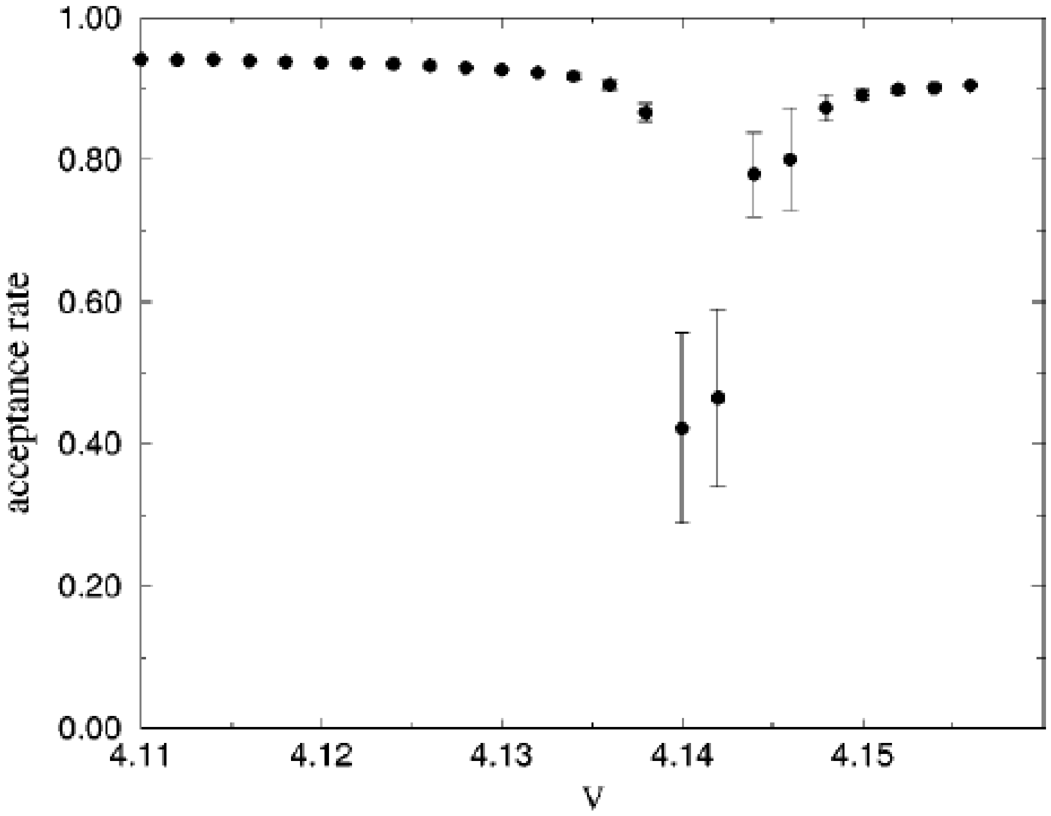
Parallel Tempering





Parallel Tempering





Bond-order-wave phase and quantum phase transitions in the one-dimensional extended Hubbard model
Pinaki Sengupta, Anders W. Sandvik, and David K. Campbell
Phys. Rev. B **65**, 155113 (2002)