Notes

Worm algorithm

Blomquist, Emil
emilbl@kth.se

May 7, 2018

Contents

Theory

Hamiltonian

The Bose-Hubbard Hamiltonian for the single condensate indexed a

$$\hat{H}_a = -\sum_{\langle i,j \rangle} t_{i,j}\, \hat{c}^\dagger_{a,i} \hat{c}_{a,j} - \sum_i \mu_{a,i}\, \hat{n}_{a,i} + \sum_i \frac{U_a}{2} \hat{n}_{a,i}(\hat{n}_{a,i} - 1) \tag{1.1}$$

Inter-component interaction

$$\hat{H}_{\text{int}} = \sum_i \sum_{a>b} U_{a,b}\, \hat{n}_{a,i} \hat{n}_{b,i} \tag{1.2}$$

Worm operators in order for the discontinuities in the partition function world lines (= Green's functions sector) to be well defined

$$\hat{H}_{\text{worm}} = \sum_i \sum_a \eta_{a,i} \left(\hat{c}^\dagger_{a,i} + \hat{c}_{a,i} \right) \tag{1.3}$$

Hence the full Hamiltonian becomes

$$\hat{H} = \sum_a \hat{H}_a + \hat{H}_{\text{int}} + \hat{H}_{\text{worm}} \tag{1.4}$$

However, by absorbing some of the intra-component on-site interaction into the chemical potential

$$\mu_{a,i} \to \mu'_{a,i} = \mu_{a,i} + \tfrac{1}{2} U_a \tag{1.5}$$

Refer to this quantity as $V_{a,i}$

Also $x_{a,i} \to x_{i,a}$ since it's that way in the code?

and defining $U_{aa} = U_a/2$ this Hamiltonian may expressed in the more convenient form

$$\begin{aligned}\hat{H} = &- \sum_a \sum_{\langle i,j \rangle} t_{i,j}\, \hat{c}^\dagger_{a,i} \hat{c}_{a,j} \\ &- \sum_a \sum_i \mu'_{a,i}\, \hat{n}_{a,i} \\ &+ \sum_{a \geq b} \sum_i U_{a,b}\, \hat{n}_{a,i} \hat{n}_{b,i} \\ &+ \sum_i \sum_a \eta_{a,i} \left(\hat{c}^\dagger_{a,i} + \hat{c}_{a,i} \right)\end{aligned} \tag{1.6}$$

Super-counter-fluid phase

In the super-counter-fluid (SCF) phase, try a Bogoliubov transformation (?)

$$\hat{a} = \alpha \hat{c}_1 + \beta \hat{c}^\dagger_2 \,, \;\; \hat{b} = \gamma \hat{c}_1 + \delta \hat{c}_2 \tag{1.7}$$

$$|\alpha|^2 + |\beta|^2 = |\gamma|^2 + |\delta|^2 = 1 \,, \; + \ldots \tag{1.8}$$

so that

$$[\hat{a}, \hat{a}^\dagger] = [\hat{b}, \hat{b}^\dagger] = 1 \,, \;\; [\hat{a}, \hat{b}^\dagger] = [\hat{a}, \hat{b}] = 0 \tag{1.9}$$

Maybe we would actually like to have $\hat{a} = \hat{c}_1 \hat{c}^\dagger_2$. Nah, thats bullshit...

Lattice path integral formulation

Derivation

Following the derivation [**Sellin**, 1, 2]

Using the Fock basis set of occupation numbers $|\alpha_m\rangle = |\{n_{a,i}\}\rangle$ the potential energy part

$$\hat{V} = - \sum_a \sum_i \mu'_{a,i}\, \hat{n}_{a,i} + \sum_{a \geq b} \sum_i U_{a,b}\, \hat{n}_{a,i} \hat{n}_{b,i} \tag{1.10}$$

of the Hamiltonian becomes diagonal. The rest of the Hamiltonian, referred to as $T \coloneqq H - V$ (not to be confused with temperature), becomes in this representation completely off-diagonal. That is,

$$\hat{V}|\alpha_n\rangle \coloneqq V_{\alpha_n} |\alpha_n\rangle \,, \quad \hat{T}|\alpha_n\rangle = \sum_{\alpha_m} |\alpha_m\rangle \langle \alpha_m | \hat{T} | \alpha_n \rangle \coloneqq \sum_{\alpha_m} T^{\alpha_m}_{\alpha_n} |\alpha_m\rangle \tag{1.11}$$

where $T^{\alpha_n}_{\alpha_n} \equiv 0 \; \forall \alpha_n$.

We wish to express the statistical operator

$$\hat{\rho}(\beta) \coloneqq e^{-\beta \hat{H}} \,, \tag{1.12}$$

as a perturbation series in terms of T. In order to achieve this we observe that ρ satisfies

$$\frac{\partial}{\partial t} \left[e^{t\hat{V}} \, \hat{\rho}(t) \right] = -e^{t\hat{V}} \hat{T} \hat{\rho}(t) \,. \tag{1.13}$$

Integrating t from 0 to τ together with the definition (1.12) one obtains

$$\hat{\rho}(\tau) = e^{-\tau \hat{V}} \left[1 - \int_0^\tau \mathrm{d}\tau \, e^{\tau \hat{V}} \hat{T} \hat{\rho}(\tau) \right] . \tag{1.14}$$

By repeated self insertion the perturbative Dyson series is revealed

$$\hat{\rho}(\tau_0) = e^{-\tau_0 \hat{V}} \sum_{n=0}^{\infty} (-1)^n \prod_{i=0}^{n} \int_0^{\tau_i} \mathrm{d}\tau_{i+1} \, \hat{T}(\tau_{i+1}) \tag{1.15}$$

where $\hat{T}(\tau) \coloneqq e^{\tau \hat{V}} \hat{T} e^{-\tau \hat{V}}$ (interaction picture representation). The integrand of order n in this series then have the form

$$\hat{O}_n = e^{-(\tau_0 - \tau_1)\hat{V}} \hat{T} e^{-(\tau_1 - \tau_2)\hat{V}} \hat{T} \cdots \hat{T} e^{-(\tau_{n-1} - \tau_n)\hat{V}} \hat{T} e^{-\tau_n \hat{V}} \tag{1.16}$$

whose expectation value with respect to the Fock state $|\alpha_m\rangle$ may be expressed in terms of the matrix elements defined in Eq. (1.11) as follows

$$\begin{aligned} \langle \alpha_m | \hat{O}_n | \alpha_m \rangle &= \sum_{\alpha_2} \cdots \sum_{\alpha_n} T^{\alpha_m}_{\alpha_2} T^{\alpha_2}_{\alpha_3} \cdots T^{\alpha_{n-1}}_{\alpha_n} T^{\alpha_n}_{\alpha_m} \\ &\quad \times \exp\left\{ -(\tau_0 - \tau_1) V_{\alpha_m} \cdots - (\tau_{n-1} - \tau_n) V_{\alpha_n} - \tau_n V_{\alpha_m} \right\} \\ &= \sum_{\alpha_1} \cdots \sum_{\alpha_{m-1}} T^{\alpha_m}_{\alpha_1} T^{\alpha_1}_{\alpha_2} \cdots T^{\alpha_{m-2}}_{\alpha_{m-1}} T^{\alpha_{m-1}}_{\alpha_m} \exp\Big\{ - \int_0^{\tau_0} \mathrm{d}\tau \, V\big[\alpha(\tau)\big] \Big\} \end{aligned} \tag{1.17}$$

where in the final equality we have renamed the dummy Fock states indices $n \to m - 1$ and approximated the sum in the exponent with an integral by taking the continuum limit $\alpha_n \to \alpha(\tau)$.

Using Eq. (1.15) and (1.17) the partition function may be expressed as

$$
\begin{aligned}
Z &= \sum_{\alpha_n} \langle \alpha_n | \hat{\rho}(\beta) | \alpha_n \rangle \\
&= \sum_{n=0}^{\infty} \Big(\prod_{i=1}^{n} \sum_{\alpha_i} \Big) \int_0^{\beta} \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \cdots \int_0^{\tau_n} \mathrm{d}\tau_n \\
&\times (-1)^n \, T^{\alpha_n}_{\alpha_1} T^{\alpha_1}_{\alpha_2} \cdots T^{\alpha_{n-2}}_{\alpha_{n-1}} T^{\alpha_{n-1}}_{\alpha_n} \exp\Big\{ - \int_0^{\beta} \mathrm{d}\tau \, V\big[\alpha(\tau)\big] \Big\} .
\end{aligned}
\tag{1.18}
$$

Since the integrands are real and positive they may be thought of as worldline configuration weights and may be sampled using Monte Carlo methods. Due to the periodic boundary conditions $\alpha(\tau = 0) = \alpha(\tau = \beta)$ the only nonzero contributing worldlines must be closed paths so that

$$
\begin{aligned}
Z &= \sum_{\text{c.p.}} W \\
W &= (-1)^n \, \mathrm{d}\tau_1 \cdots \mathrm{d}\tau_n \, T^{\alpha_n}_{\alpha_1} T^{\alpha_1}_{\alpha_2} \cdots T^{\alpha_{n-2}}_{\alpha_{n-1}} T^{\alpha_{n-1}}_{\alpha_n} \exp\Big\{ - \int_0^{\beta} \mathrm{d}\tau \, V\big[\alpha(\tau)\big] \Big\}
\end{aligned}
\tag{1.19}
$$

No two particles regardless of component could jump/be created/be removed at the same time with the current expression of T. This follows from analyzing $\hat{T} \, |\alpha_m\rangle$ where $\hat{T} = \sum_a \hat{T}^{(a)}$ and $|\alpha_m\rangle = \prod_a |\alpha_m^{(a)}\rangle$ and a labels the different components.

Observables

Kinetic energy

For a general kinetic energy operator $\hat{K} = \sum_i t_i \hat{O}_i$ where $\hat{O}_i$ is any off-diagonal jump operator it is possible to show that the statistical ensemble average is proportional to the average number of total kinks $\langle N^{\text{kinks}} \rangle$.

$$
\langle \hat{K} \rangle = \sum_i t_i \langle \hat{O}_i \rangle \tag{1.20}
$$

where

$$
\begin{aligned}
\langle \hat{O}_i \rangle &= \frac{1}{Z} \mathrm{Tr} \Big\{ \hat{O}_i \, e^{-\beta \hat{H}} \Big\} \\
&= \frac{1}{Z} \mathrm{Tr} \Big\{ \hat{O}_i \, \exp\big\{ - \beta (t_i \hat{O}_i + \text{terms independent of } t_i) \big\} \Big\} \\
&= -\frac{1}{\beta} \frac{1}{Z} \frac{\partial Z}{\partial t_i}
\end{aligned}
\tag{1.21}
$$

so that

$$\langle \hat{K} \rangle = -\frac{1}{\beta} \frac{1}{Z} \sum_i t_i \frac{\partial Z}{\partial t_i} \,. \tag{1.22}$$

Using Eq. (1.19) the partition function may be expressed as

$$Z = \sum_{\text{c.p.}} W = \sum_{\text{c.p.}} W' \prod_j t_j^{N_j} \tag{1.23}$$

where everything but the jump factors t_i have been factored out into W'. Here the exponents N_j correspond precisely to the number of kinks of type t_j. From this it is then obvious that

$$t_i \frac{\partial W}{\partial t_i} = N_i W \tag{1.24}$$

which is substituted into Eq. (1.22)

$$\begin{aligned} \langle \hat{K} \rangle &= -\frac{1}{\beta} \frac{1}{Z} \sum_i t_i \frac{\partial Z}{\partial t_i} \\ &= -\frac{1}{\beta} \frac{1}{Z} \sum_{\text{c.p.}} \sum_i N_i W \\ &= -\frac{1}{\beta} \frac{1}{Z} \sum_{\text{c.p.}} N^{\text{kinks}} W \\ &= -\frac{1}{\beta} \langle N^{\text{kinks}} \rangle \end{aligned} \tag{1.25}$$

Particle number

We would like to derive an expression for the expectation value of the number of particles in component a at site i, i.e. $\langle \hat{n}_{a,i} \rangle$. Analogously to Eq. (1.21) we have

$$\langle \hat{n}_{a,i} \rangle = \frac{1}{\beta} \frac{1}{Z} \frac{\partial Z}{\partial \mu_{a,i}} \tag{1.26}$$

and similarly to Eq. (1.23)

$$Z = \sum_{\text{c.p.}} W' \, \exp\left\{ \int_0^\beta \mathrm{d}\tau \, \mu_{a,i} n_{a,i}(\tau) \right\} \tag{1.27}$$

where W' is the rest of W, independent of $\mu_{a,i}$. It is then trivial to show that

$$\langle \hat{n}_{a,i} \rangle = \left\langle \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \, n_{a,i}(\tau) \right\rangle \tag{1.28}$$

Following the derivation above but exchanging $\mu_{a,i} \to U_{a,b,i}$ is straight forward to derive

$$\langle \hat{n}_{a,i} \hat{n}_{b,i} \rangle = \left\langle \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \, n_{a,i}(\tau) n_{b,i}(\tau) \right\rangle . \tag{1.29}$$

Potential energy

Substituting the expressions for the expectation value of particle numbers, the expectation value of the potential value follow

in the original Hamiltonian

$$\begin{aligned}
\langle \hat{V} \rangle &= -\sum_a \sum_i \mu_{a,i} \langle \hat{n}_{a,i} \rangle + \sum_a \sum_i \frac{U_a}{2} \langle \hat{n}_{a,i} (\hat{n}_{a,i} - 1) \rangle + \sum_{a>b} \sum_i U_{a,b} \langle \hat{n}_{a,i} \hat{n}_{b,i} \rangle \\
&= -\sum_a \sum_i \mu_{a,i} \left\langle \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \, n_{a,i}(\tau) \right\rangle \\
&- \sum_a \frac{U_a}{2} \left[\left\langle \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \sum_i n_{a,i}^2(\tau) \right\rangle - \left\langle \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \sum_i n_{a,i}(\tau) \right\rangle \right] \\
&+ \sum_{a>b} U_{a,b} \left\langle \frac{1}{\beta} \int_0^\beta \mathrm{d}\tau \sum_i n_{a,i}(\tau) n_{b,i}(\tau) \right\rangle
\end{aligned} \tag{1.30}$$

Metropolis-Hastings algorithm

Detailed balance

- $P(x)$: probability distribution corresponding to state x
- $P(x \to x')$: transition probability of going from state x to x'

A system in detailed balance is then required to satisfy

$$P(x) P(x \to x') = P(x') P(x \to x') \tag{1.31}$$

for every state x and x'. However, note that this is satisfied if $P(x \to x') \equiv 0$ for several states x and x'.

Ergodicity

Metropolis-Hastings algorithm

Expressing the transition probabilities as a product of a proposal and acceptance-rejection probability.

$$P(x \to x') = g(x \to x')\, A(x \to x') \tag{1.32}$$

- $g(x \to x')$: proposal distribution. From this distribution the new state x' is proposed from the current state x. Clearly this distribution might be engineered in multiple ways.
- $A(x \to x')$: acceptance-rejection conditional probability distribution of accepting the proposed state x' given x. This follows from the choice of $W(x \to x')$ and $P(x)$. **It is important that** $0 \leq A \leq 1$ **!**

Substituting this into the expression of detailed balance

$$A(x \to x') = \frac{P(x')}{P(x)} \frac{g(x' \to x)}{g(x \to x')} A(x' \to x) := R(x \to x')\, A(x' \to x) \tag{1.33}$$

which is satisfied by the Metropolis choice

$$A(x \to x') = \min\{1,\, R(x \to x')\} \tag{1.34}$$

In case of a pair of update-anti-update procedures one can set the larger of the Acceptance ratios to unity. However it is really important that it is the larger one due to the fact that $0 \leq A \leq 1$ must be fulfilled.

Bootstrap

This algorithm is incorrect and not actually bootstrap, so the text needs to be rewritten. However the implemented code is correct.

In order to estimate the uncertainty in a statistical averaged quantity $\langle A \rangle$, i.e. $\sigma(\langle A \rangle)$ one may utilize the bootstrap method.

Given a set S of N independent (not necessary) data points A_i where $i \in [0, N-1]$, pick on random a subset $s_b \subseteq S$ with $n < N$ number of elements for which the mean value $\langle A \rangle_i$ is calculated. By repeating this procedure m times, i.e $b \in [0, m-1]$ the uncertainty in $\langle A \rangle$ is estimated as

$$\sigma(\langle A\rangle) = \sqrt{\sum_i \left(\langle A\rangle - \langle A\rangle_i\right)^2} \tag{1.35}$$

where $\langle A\rangle = \sum_i \langle A\rangle_i$. A reasonable choice of n and m would be such that the data is not overused, that is, $n\,m \leq N$ with $1 \ll m \sim 100$.

Implementation

Imaginary-time discretization

Code structure

Classes

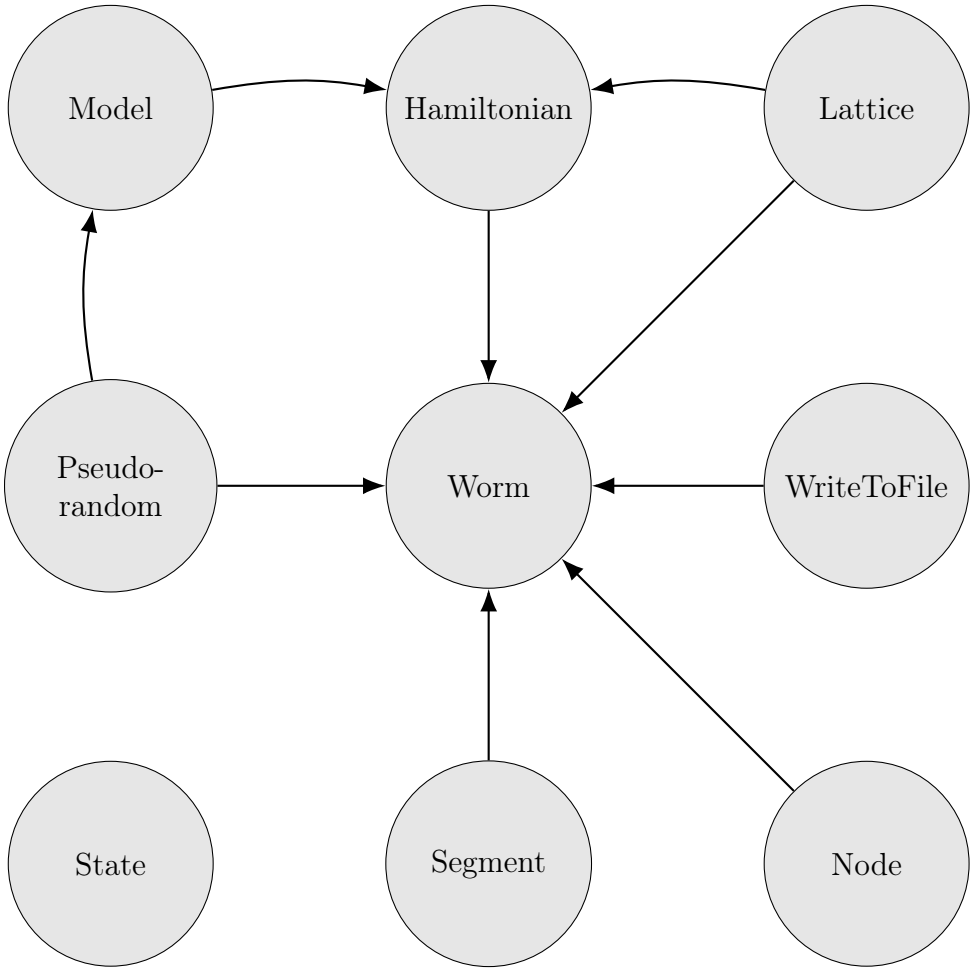


Figure 2.1: Relation between the different classes in the program. An arrow pointing onto a class indicates that this class is dependent upon the class where the arrow begun. This illustration is outdated.

State

Singleton, Global

Tells in what state the program should run, i.e. *verbose*, *debug* and/or *shutItDown* mode.

Pseudorandom

Singleton

Generates pseudorandom numbers used in *Model* and *Worm* classes

WriteToFile

Singleton

Used for saving quantities to file.

Lattice

Singleton

Contains different types of lattices.

Model

Singleton

Contains different types of models.

Hamiltonian

Singleton

Given a certain lattice and model a Hamiltonian is created and stored in an efficient way for the *Worm* algorithm class to access quickly.

Worm

Singleton

The worm algorithm.

Segment

The segments used to describe the worldline.

ETC

In order to bin observables both efficiently and exact the following quantities are being kept track of during the simulation.

- Number of particles per site and component $n_{a,i}$

```
std::vector<std::array<unsigned long long, numComps> >
```

- Total number of kinks per component N_a^{kinks}

```
std::array<unsigned, numComps>
```

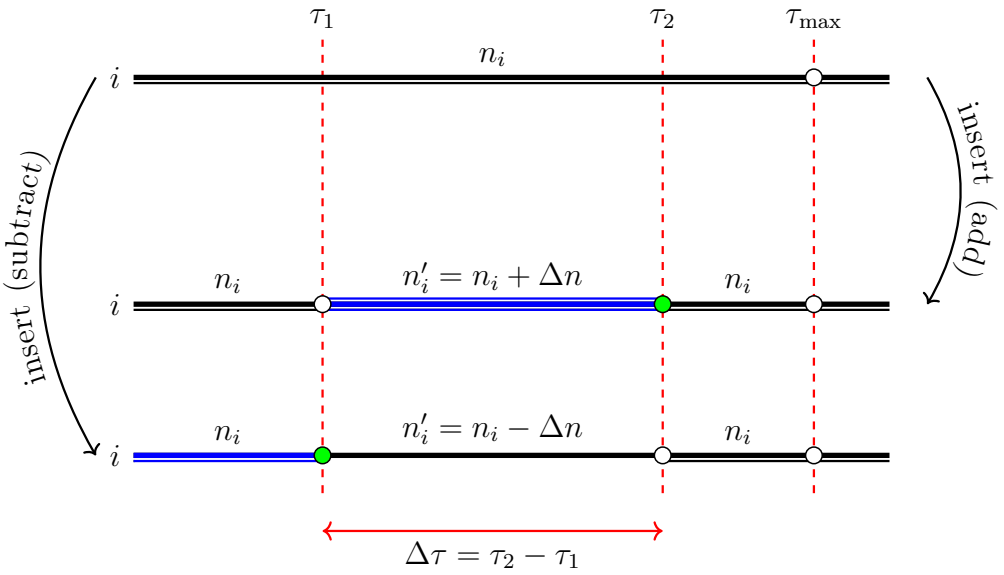
- Total number of particles squared (inter and intra component) $n_a n_b = \sum_i n_{a,i} n_{b,i}$

```
std::array<unsigned long long, numComps * (numComps + 1) / 2>
```

Update methods

For the current Hamiltonian only single particle worms are allowed.

Insert



- Δn_a: worm population of condensate indexed a
  - $\Delta n_a = 1$: particle worm in component a.
  - $\Delta n_a = -1$: hole worm in component a.
  - $\Delta n_a = 0$: no worm in component a.
- Add or subtract the worm ($+$ or $-$): $n_i' = n_i \pm \Delta n$

Weight ratio

$$\begin{aligned}\frac{W'_\mu}{W_\mu} &= \frac{\exp\left\{(\tau_2-\tau_1)\sum_a \mu_{a,i}[n_{a,i}\pm\Delta n_a]\right\}}{\exp\left\{(\tau_2-\tau_1)\sum_a \mu_{a,i} n_{a,i}\right\}} \\ &= \exp\left\{\pm\Delta\tau\sum_a \mu_{a,i}\Delta n_a\right\}\end{aligned} \tag{2.1}$$

$$\begin{aligned}\frac{W'_U}{W_U} &= \frac{\exp\left\{-(\tau_2-\tau_1)\sum_{a\geq b} U_{a,b}\,[n_{a,i}\pm\Delta n_a][n_{b,i}\pm\Delta n_b]\right\}}{\exp\left\{-(\tau_2-\tau_1)\sum_{a\geq b} U_{a,b}\,n_{a,i}n_{b,i}\right\}} \\ &= \exp\left\{-\Delta\tau\sum_{a\geq b} U_{a,b}[\Delta n_a\Delta n_b \pm n_{a,i}\Delta n_b \pm n_{b,i}\Delta n_a]\right\}\end{aligned} \tag{2.2}$$

$$\frac{W'_\eta}{W_\eta} = \ldots \tag{2.3}$$

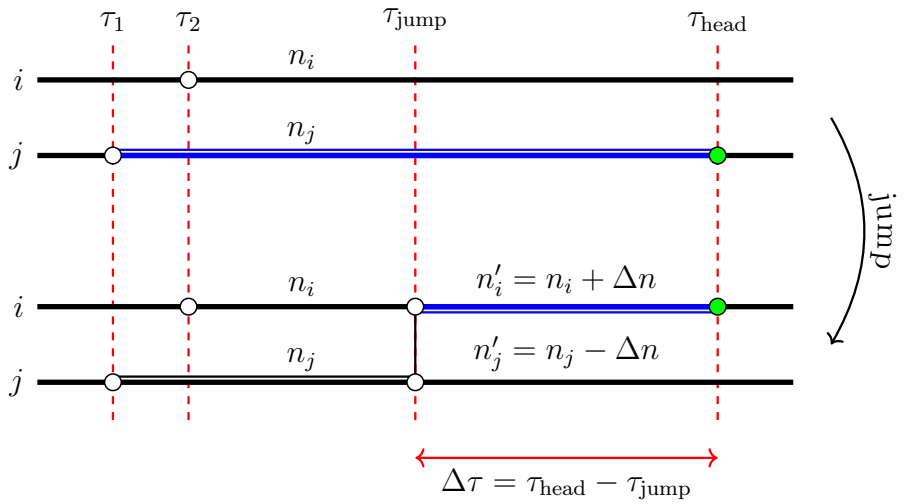
Probability distribution

$$\begin{aligned}\frac{P'}{P} &= P(i) \\ &\times P(\Delta n) \\ &\times P(\pm) \\ &\times P(\tau_1) \\ &\times P(i,\tau_1\to\tau_2) \\ &\times P(\text{ways of removing the worm (anti-add and/or anti-subtract)}\to\text{choosen one})^{-1} \\ &\times \left(\frac{W_{\text{remove}}}{\sum_i W_i}\right)^{-1}\end{aligned} \tag{2.4}$$

since $W_{\text{insert}} = 1$ in the Z-sector.

Remove (anit-insert)

Jump



- i: proposed site index of worm head
- j: current site index of worm head
- a: condensate component index
- Δn_a: worm population of condensate indexed a (possible values -1, 0, 1)
- $\Delta\tau$: length of the new segment belonging to the head (disregarding from a possible split due to crossing the $\tau = \beta$ boundary)

Weight ratio

$$\begin{aligned}
\frac{W'_\mu}{W_\mu} &= \frac{\exp\left\{\Delta\tau \sum_a [\mu_{a,i} n'_{a,i} + \mu_{a,j} n'_{a,j}]\right\}}{\exp\left\{\Delta\tau \sum_a [\mu_{a,i} n_{a,i} + \mu_{a,j} n_{a,j}]\right\}} \\
&= \exp\left\{\Delta\tau \sum_a \left[\mu_{a,i}(n_{a,i} + \Delta n_a) + \mu_{a,j}(n_{a,j} - \Delta n_a) - \mu_{a,i} n_{a,i} - \mu_{a,j} n_{a,j}\right]\right\} \qquad (2.5) \\
&= \exp\left\{\Delta\tau \sum_a \Delta n_a \left[\mu_{a,i} - \mu_{a,j}\right]\right\}
\end{aligned}$$

$$
\begin{aligned}
\frac{W'_U}{W_U} &= \frac{\exp\left\{-\Delta\tau \sum_{a\geq b} U_{a,b}[n'_{a,i}n'_{b,i} + n'_{a,j}n'_{b,j}]\right\}}{\exp\left\{-\Delta\tau \sum_{a\geq b} U_{a,b}[n_{a,i}n_{b,i} + n_{a,j}n_{b,j}]\right\}} \\
&= \exp\Big\{ -\Delta\tau \sum_{a\geq b} U_{a,b}\big[(n_{a,i}+\Delta n_a)(n_{b,i}+\Delta n_b) \\
&\qquad + (n_{a,j}-\Delta n_a)(n_{b,j}-\Delta n_b) - n_{a,i}n_{b,i} - n_{a,j}n_{b,j}\big]\Big\} \\
&= \exp\left\{-\Delta\tau \sum_{a\geq b} U_{a,b}\left[2\Delta n_a\Delta n_b + n_{a,i}\Delta n_b + n_{b,i}\Delta n_a - n_{a,j}\Delta n_b - n_{b,j}\Delta n_a\right]\right\} \\
&= \exp\left\{-\Delta\tau \sum_{a\geq b} U_{a,b}\left[2\Delta n_a\Delta n_b + \Delta n_a\left(n_{b,i}-n_{b,j}\right) + \Delta n_b\left(n_{a,i}-n_{a,j}\right)\right]\right\}
\end{aligned}
\tag{2.6}
$$

$$
\begin{aligned}
\frac{W'_t}{W_t} &= \frac{\prod_a \Big(\overbrace{t_{i,j}\sqrt{n'_{a,i}n_{a,j}}\,\delta_{\Delta n_a,1}}^{\text{particle worm}} + \overbrace{t_{j,i}\sqrt{n'_{a,j}n_{a,i}}\,\delta_{\Delta n_a,-1}}^{\text{hole worm}} \Big)}{1} \\
&= \prod_a \left(t_{i,j}\sqrt{(n_{a,i}+\Delta n_a)n_{a,j}}\,\delta_{\Delta n_a,1} + t_{j,i}\sqrt{(n_{a,j}-\Delta n_a)n_{a,i}}\,\delta_{\Delta n_a,-1} \right) \\
&= \prod_a \left(t_{i,j}\sqrt{(n_{a,i}+1)n_{a,j}}\,\delta_{\Delta n_a,1} + t_{j,i}\sqrt{(n_{a,j}+1)n_{a,i}}\,\delta_{\Delta n_a,-1} \right)
\end{aligned}
\tag{2.7}
$$

$$
\begin{aligned}
\frac{W'_\eta}{W_\eta} &= \frac{\prod_a \eta_a \Big(\overbrace{\sqrt{n'_{a,i}}\,\delta_{\Delta n_a,1}}^{\text{particle worm}} + \overbrace{\sqrt{n'_{a,i}+1}\,\delta_{\Delta n_a,-1}}^{\text{hole worm}} \Big)}{\prod_a \eta_a \Big(\underbrace{\sqrt{n_{a,j}}\,\delta_{\Delta n_a,1}}_{\text{particle worm}} + \underbrace{\sqrt{n_{a,j}+1}\,\delta_{\Delta n_a,-1}}_{\text{hole worm}} \Big)} \\
&= \prod_a \frac{\sqrt{n_{a,i}+\Delta n_a}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,i}+\Delta n_a+1}\,\delta_{\Delta n_a,-1}}{\sqrt{n_{a,j}}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,j}+1}\,\delta_{\Delta n_a,-1}} \\
&= \prod_a \frac{\sqrt{n_{a,i}+1}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,i}}\,\delta_{\Delta n_a,-1}}{\sqrt{n_{a,j}}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,j}+1}\,\delta_{\Delta n_a,-1}}
\end{aligned}
\tag{2.8}
$$

Probability distribution

$$
\begin{aligned}
\frac{P'}{P} &= P(j\to i) \\
&\quad \times P(\max\{\tau_1,\,\tau_2\},\, \tau_{\text{head}} \to \tau_{\text{jump}}) \\
&\quad \times \frac{W_{\text{jump}}}{W_{\text{anti-jump}}}
\end{aligned}
\tag{2.9}
$$

where W_i is the probability weight of update procedure i.

Anti-jump

The anti-update procedure to adding a worm is referred to as removing the worm backwards (the head is reversing into the tail) as opposed to removing the worm forward (the head is reaching the tail going forward) which clearly is the anti-update procedure to insertion via subtraction.

Reconnect

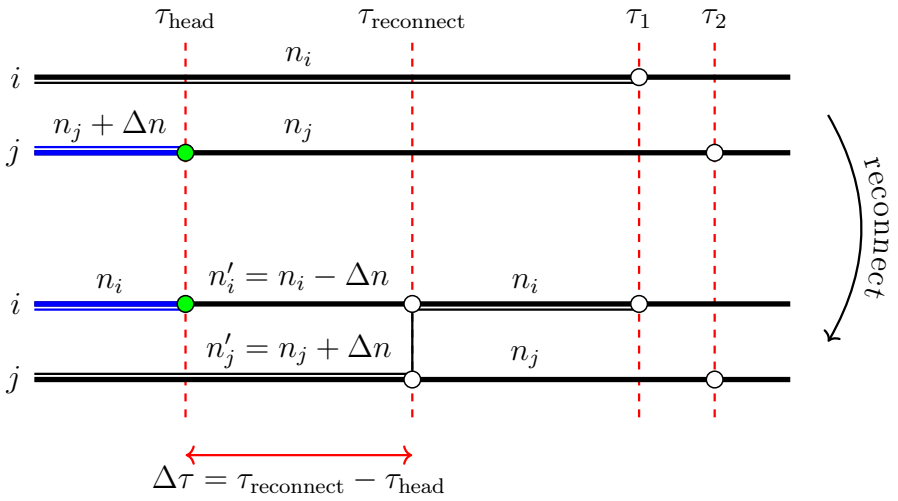


Figure 2.2: Steal Δn population from the i^{th} lattice site to fill the discontinuity between τ_{head} and $\tau_{\text{reconnect}}$.

Weight ration

The calculation of the contribution from the jump is analogous to the one from the jump update procedure but with $n_{a,i} \leftrightarrow n_{a,j}$ everywhere (primed and unprimed quantities) so that

$$\frac{W_t'}{W_t} = \prod_a \left(t_{i,j} \sqrt{n_{a,i}(n_{a,j}+1)}\, \delta_{\Delta n_a,1} + t_{j,i} \sqrt{n_{a,j}(n_{a,i}+1)}\, \delta_{\Delta n_a,-1} \right) . \tag{2.10}$$

Also the contributions from the chemical potential and the on-site interaction are precisely the ones for the jump update procedure but with $i \leftrightarrow j$, i.e.

$$\frac{W_\mu'}{W_\mu} = \exp\left\{ \Delta\tau \sum_a \Delta n_a \left[\mu_{a,j} - \mu_{a,i} \right] \right\} \tag{2.11}$$

and

$$\frac{W'_U}{W_U} = \exp\left\{ -\Delta\tau \sum_{a\geq b} U_{a,b}\left[2\Delta n_a \Delta n_b + \Delta n_a\left(n_{b,j} - n_{b,i}\right) + \Delta n_b\left(n_{a,j} - n_{a,i}\right)\right]\right\}. \quad (2.12)$$

Finally the worm operator contribution, also similar to that of the jump update procedure

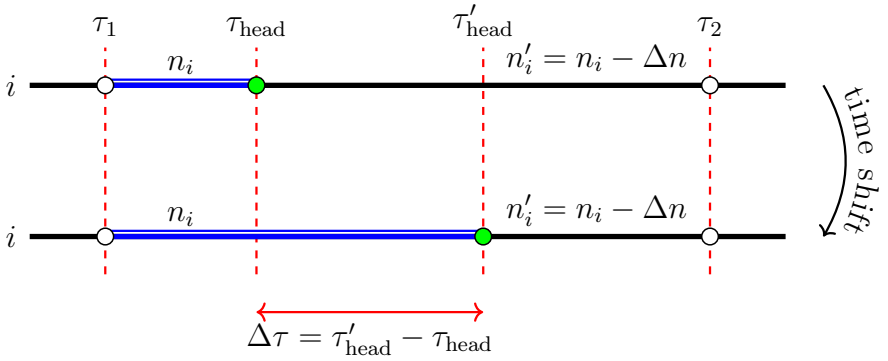
$$\begin{aligned}
\frac{W'_\eta}{W_\eta} &= \frac{\prod_a \eta_a\Big(\overbrace{\sqrt{n_{a,i}}\,\delta_{\Delta n_a,1}}^{\text{particle worm}} + \overbrace{\sqrt{n_{a,i}+1}\,\delta_{\Delta n_a,-1}}^{\text{hole worm}}\Big)}{\prod_a \eta_a\Big(\underbrace{\sqrt{n'_{a,j}}\,\delta_{\Delta n_a,1}}_{\text{particle worm}} + \underbrace{\sqrt{n'_{a,j}+1}\,\delta_{\Delta n_a,-1}}_{\text{hole worm}}\Big)} \\
&= \prod_a \frac{\sqrt{n_{a,i}}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,i}+1}\,\delta_{\Delta n_a,-1}}{\sqrt{n_{a,j}+\Delta n_a}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,j}+\Delta n_a+1}\,\delta_{\Delta n_a,-1}} \\
&= \prod_a \frac{\sqrt{n_{a,i}}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,i}+1}\,\delta_{\Delta n_a,-1}}{\sqrt{n_{a,j}+1}\,\delta_{\Delta n_a,1} + \sqrt{n_{a,j}}\,\delta_{\Delta n_a,-1}}\,.
\end{aligned} \quad (2.13)$$

Probability distribution

$$\begin{aligned}
\frac{P'}{P} &= P(j \to i) \\
&\times P(\tau_{\text{head}},\, \min\{\tau_1,\, \tau_2\} \to \tau_{\text{reconnect}}) \\
&\times \frac{W_{\text{reconnect}}}{W_{\text{anti-reconnect}}}
\end{aligned} \quad (2.14)$$

Anti-reconnect

Time shift



Weight ratio

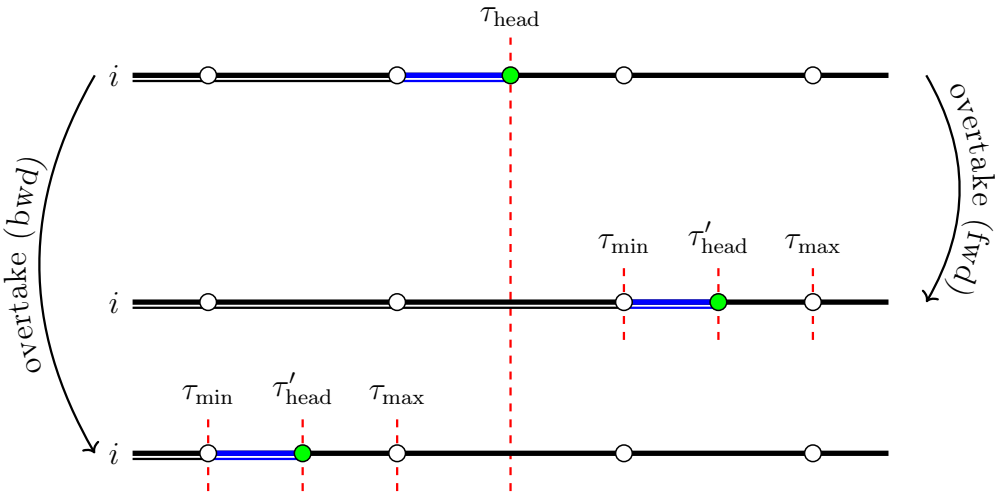
$$\begin{aligned}\frac{W'_\mu}{W_\mu} &= \frac{\exp\left\{(\tau'_{\text{head}}-\tau_1)\sum_a \mu_{a,i} n_{a,i} + (\tau_2-\tau'_{\text{head}})\sum_a \mu_{a,i} n'_{a,i}\right\}}{\exp\left\{(\tau_{\text{head}}-\tau_1)\sum_a \mu_{a,i} n_{a,i} + (\tau_2-\tau_{\text{head}})\sum_a \mu_{a,i} n'_{a,i}\right\}} \\ &= \exp\left\{\Delta\tau \sum_a \mu_{a,i} n_{a,i} - \Delta\tau \sum_a \mu_{a,i}[n_{a,i}-\Delta n_a]\right\} \\ &= \exp\left\{\Delta\tau \sum_a \mu_{a,i} \Delta n_a\right\}\end{aligned} \tag{2.15}$$

$$\begin{aligned}\frac{W'_U}{W_U} &= \frac{\exp\left\{-(\tau'_{\text{head}}-\tau_1)\sum_{a\geq b} U_{a,b}\, n_{a,i} n_{b,i} - (\tau_2-\tau'_{\text{head}})\sum_{a\geq b} U_{a,b}\, n'_{a,i} n'_{b,i}\right\}}{\exp\left\{-(\tau_{\text{head}}-\tau_1)\sum_{a\geq b} U_{a,b}\, n_{a,i} n_{b,i} - (\tau_2-\tau_{\text{head}})\sum_{a\geq b} U_{a,b}\, n'_{a,i} n'_{b,i}\right\}} \\ &= \exp\left\{-\Delta\tau \sum_{a\geq b} U_{a,b}\, n_{a,i} n_{b,i} + \Delta\tau \sum_{a\geq b} U_{a,b}\,[n_{a,i}-\Delta n_a][n_{b,i}-\Delta n_b]\right\} \\ &= \exp\left\{-\Delta\tau \sum_{a\geq b} U_{a,b}[n_{a,i}\Delta n_b + n_{b,i}\Delta n_a - \Delta n_a \Delta n_b]\right\}\end{aligned} \tag{2.16}$$

Probability distribution

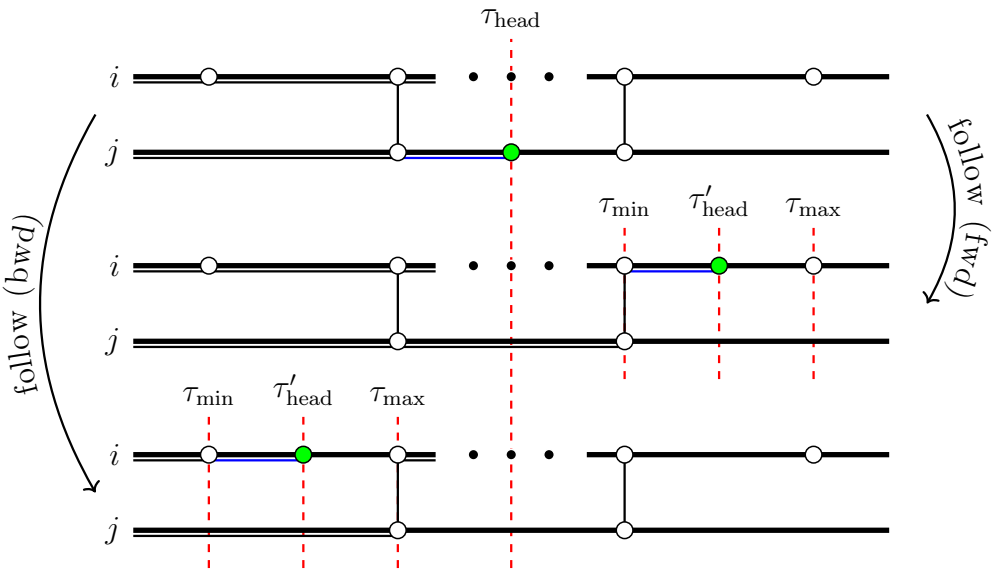
$$\frac{P'}{P} = \frac{P(\tau_1,\, \tau_2 \to \tau'_{\text{head}})}{P(\tau_1,\, \tau_2 \to \tau_{\text{head}})} \tag{2.17}$$

Overtake



Barely go into the previous or next segment whilst staying on the same site. Care needs to be taken to the fact that this might cause discontinuities in particle number which of course is not allowed.

Follow



Follow the current segment forward or backwards via a jump into another lattice site. Must not allow for two of the same particles to jump simultaneously.

How to handle zero net transfer of particles in a particular component but there being a jump from $i \to j$ and $j \to i$ simultaneous? Presumably this should count as no jump since two events occurring simultaneously in the same component really isn't allowed. The reason for allowing the same across components is that the jump contribution from component a is only dependent on the number of particles in component a at that instant, and not dependent on the number of particles in component $b \neq a$. Of course it is really unlikely for two such events to occur simultaneously, but this is merely an approximation since the time is discretized. In reality, if one were to "zoom" in, one would probably find them separated by a small distance in time $0 < \epsilon \ll 1$. The error arising from such a coarse grinding is of the order of $\exp(C\epsilon) \sim \epsilon$ since typically $C \sim 1$. In spin-orbit interactions this is not so clear any more.

That being said, it is not possible to completely "unfollow" a jump (basically an anti-jump or an anti-reconnect) because that would go against the detail balance. After such an update there would be no track of the jump having been there in the first place, so there would be no possibility of going back with the same update procedure. This goes against the criterion of detailed balance. Therefore this update procedure will never be allowed in the one component case.

Notes

In many of these update procedures certain choices of parameters would result in an erroneous worm configuration. If such is the case, the update procedure is immediately canceled since the transition probability from a correct to an erroneous state should be identically zero. This will of course not affect the transition probability going to a allowed worm configuration.

Value of η

when inserting a worm the acceptance ratio is proportional against

$$A(Z \to G) \propto \frac{\eta^2}{P(i)\, P(\tau_{\text{tail}})} = \eta^2\, N\beta \quad \Leftarrow \quad \eta = 1/sqrtN\beta \tag{2.18}$$

where N is the number of sites and $P(\tau_1)$ is the uniform interval of selecting τ_{tail} for the tail. For all of this to be true the probability of choosing τ_{head} should of course be an exponential distribution.

There should not be one η for each component. Rather one for each end of the worm. For a n-component system it would otherwise be difficult to optimize the insertion of variable number component worms.

Debug

Allowing only for one-component particle worm

Independence of η

Scale

Given $\langle N \rangle$, $\langle E_K \rangle$, $\langle E_\mu \rangle$ and $\langle E_U \rangle$ obtained using the parameter t, μ, U, η and β

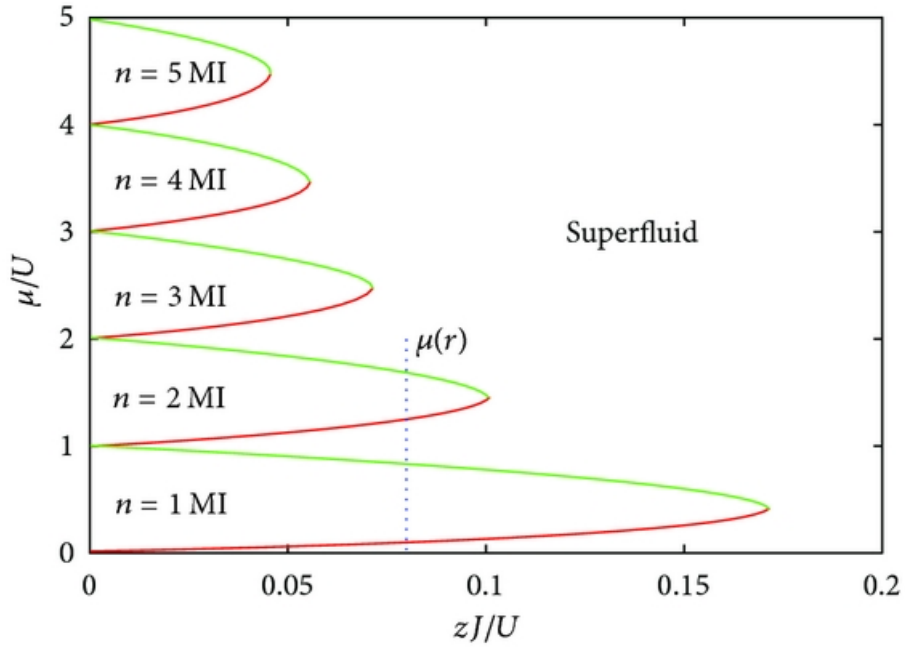


Figure 2.3: Mott lobes for some type of Bose-Hubbard model. For us $zJ = t$.

Bibliography

[1] R.P. Feynman. *Statistical Mechanics: A Set Of Lectures*. Advanced Books Classics. Avalon Publishing, 1998. ISBN: 9780813346106. URL: https://books.google.se/books?id=iQ9uDgAAQBAJ.

[2] Boris Svistunov. *Superfluid states of matter*. Boca Raton, FL: CRC Press, Taylor & Francis Group, 2015. ISBN: 9781439802755.